(19) World Intellectual Property **Organization**

International Bureau





(43) International Publication Date 22 January 2004 (22.01.2004)

PCT

(10) International Publication Number WO 2004/008554 A2

(51) International Patent Classification⁷: 51/30

H01L 51/20,

(21) International Application Number:

PCT/GB2003/003035

(22) International Filing Date: 14 July 2003 (14.07.2003)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:

0216154.5 12 July 2002 (12.07.2002) GB

- (71) Applicant (for all designated States except US): ELAM-LIMITED [GB/GB]; 103 Borough Road, London SE1 OAA (GB).
- (72) Inventors; and
- (75) Inventors/Applicants (for US only): KATHIRGA-MANATHAN, Poopathy [GB/GB]; The Little Lancaster House, 1 Lancaster Road, North Harrow HA2 7NN (GB). ANTIPÁN-LARA, Juan [CL/GB]; 29 Jenner Road, London N16 7SB (GB). PARTHEEPAN, Arumugam [GB/GB]; 26 Eldertree Way, Mitcham, Surrey CR4 1AG (GB).

- (74) Agent: COHEN, Alan, Nicol; 2 Grove Place, Tatsfield, Westerham, Kent TN16 2BB (GB).
- (81) Designated States (national): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW.
- (84) Designated States (regional): ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

without international search report and to be republished upon receipt of that report

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: METAL CHELATES

(57) Abstract: A photovoltaic device which uses a metal chelate as the photovoltaic element.

- 1 -

Metal Chelates

The present invention relates to photovoltaic devices and elements useful in such devices.

5

10

Photovoltaic devices, i.e. solar cells, are capable of converting solar radiation into useable electrical energy. The energy conversion occurs as a result of what is well known in the solar cell field as the photovoltaic effect. Solar radiation impinging on a solar cell and absorbed by an active region generates electrons and holes. The electrons and holes are separated by a built-in electric field, for example a rectifying junction, in the solar cell. This separation of electrons and holes results in the generation of an electrical current as explained below. For example, a built-in electric field can be generated in a solar cell by an active semiconductor layer with regions of P-type, intrinsic and N-type hydrogenated amorphous silicon. A built-in electric field can also be generated in a solar cell by, for example, a Schottky barrier. The electrons generated at the metal (Schottky barrier) semiconductor body junction flow towards the semiconductor body.

20

15

A typical simple photovoltaic solar cell comprises an electrically conductive substrate layer; a semiconductor body deposited upon said substrate layer and a transparent conductive layer over at least a portion of said semiconductor body for facilitating collection of electrical current produced by the photovoltaic cell.

25

The electrons generated in the intrinsic region, by absorption of solar radiation of the appropriate bandgap, produce electron-hole pairs. The separation of the electron-hole pairs with the electrons flowing toward the region of N-type conductivity, and the holes flowing toward the region of P-type conductivity, creates the photovoltage and photocurrent of the cell.

30

The photocurrent output of a solar cell is maximized by increasing the total number of photons of differing energy and wavelength which are absorbed by the

- 2 -

semiconductor material. The solar spectrum roughly spans the region of wavelengths from about 300 nanometers to about 2200 nanometers, which corresponds to from about 4.2 eV to about 0.59 eV, respectively. The portion of the solar spectrum which is absorbed by the solar cell is determined by the size of the bandgap energy of the semiconductor material. In the past, solar cells were fabricated from single crystal materials such as gallium arsenide, which has a bandgap energy of about 1.45 eV, or crystalline silicon, C-Si, which has a bandgap energy of about 1.1 eV. Solar radiation having an energy less than the bandgap energy is not absorbed by the semiconductor material, and thus does not contribute to the generation of the photocurrent output of the cell.

5

10

15

20

25

30

Semiconductor materials such as GaAs and C-Si have been utilized together in solar cells to increase the overall conversion of solar energy into electrical energy. However, problems are encountered when different semiconductor materials are used in the same solar cell. One solution to the problem of fabricating a solar cell structure with different semiconductor materials was to use filters to reflect light of the appropriate wavelength onto a solar cell of the first material and transmit the non-absorbed light to a cell of the second semiconductor material. A second solution used semiconductor materials of differing bandgaps which could be epitaxially grown on one another, such as aluminum gallium arsenide, gallium arsenide, and gallium phosphide structures. Both these systems have been loosely called tandem junction solar cells. A third alternative was to stack individual solar cells of differing bandgap energies and connect the cells in series. These three alternatives are either cumbersome, expensive and/or bulky. A description of photovoltaic cells and their operation is disclosed in a paper by Jean-Michel Nunzi in C.R.Physique 3 (2002) 523-542.

We have found that a photovoltaic device can be made using metal chelates such as a rare earth or non rare earth metal chelate or a mixture of rare earth metal chelates as the photovoltaic element in place of the prior art semi conductors.

Rare earth chelates are known which fluoresce in ultra violet radiation and A. P. Sinha (Spectroscopy of Inorganic Chemistry Vol. 2 Academic Press 1971) describes several classes of rare earth chelates with various monodentate and bidentate ligands.

5

WO 2004/008554

Group III A metals and lanthanides and actinides with aromatic complexing agents have been described by G. Kallistratos (Chimica Chronika, New Series, 11, 249-266 (1982)). This reference specifically discloses the Eu(III), Tb(III), U(III) and U(IV) complexes of diphenyl-phosponamidotriphenyl-phosphoran.

10

30

EP 0556005A and 0744451A also disclose fluorescent chelates of transition or lanthanide or actinide metals.

Patent application WO98/58037 describes a range of lanthanide complexes which can be used in electroluminescent devices which have improved properties and give better results. Patent Applications PCT/GB98/01773, PCT/GB99/03619, PCT/GB99/04030, PCT/GB99/04024, PCT/GB99/04028, PCT/GB00/00268 describe electroluminescent complexes, structures and devices using rare earth chelates.

Hitherto such rare earth metal chelates have not been used in photovoltaic devices.

According to the invention there is provided a photovoltaic device comprising a metal chelate as the photovoltaic element.

The invention also provides a photovoltaic device which comprises sequentially (i) a first electrode comprising a metal, (ii) the photovoltaic element and (iii) a second electrode in which the photovoltaic element comprises a metal chelate.

By photovoltaic element is meant a compound which will generate electrons and holes when exposed to light.

- 4 -

The metal chelates can absorb light of a specific wavelength or wavelengths depending on the metal and ligands used and, as the photocurrent output of a solar cell is maximized by increasing the total number of photons of differing energy and wavelength which are absorbed by the semiconductor material, by having a plurality of layers of different metal chelates which absorb light at different wavelengths, a wide range of the visible spectrum can be used. Metal chelates can also absorb light in the infra-red, ultra-violet or shorter wavelengths so improving the utilisation of sunlight and increasing the power achievable by a solar cell. Alternatively there can be several layers of metal chelates which absorb light in different parts of the spectrum.

The preferred metal chelates useful in the present invention have the formula

$$(L\alpha)_n M$$
 or $(L\alpha)_n > M \leftarrow Lp$

15

5

10

where $L\alpha$ and Lp are organic ligands, M is a metal and n is the valence state of the metal M and in which the ligands $L\alpha$ are the same or different.

There can be a plurality of ligands Lp which can be the same or different.

20

25

For example $(L_1)(L_2)(L_3)(L_.)M$ (Lp) where M is a metal e.g. rare earth, transition metal, lanthanide or an actinide and $(L_1)(L_2)(L_3)(L_...)$ are the same or different organic complexes and (Lp) is a neutral ligand. The total charge of the ligands $(L_1)(L_2)(L_3)(L_...)$ is equal to the valence state of the metal M. Where there are 3 groups $L\alpha$ which corresponds to the III valence state of M the complex has the formula $(L_1)(L_2)(L_3)M$ (Lp) and the different groups $(L_1)(L_2)(L_3)$ may be the same or different.

5

10

15

20

Lp can be monodentate, bidentate or polydentate and there can be one or more ligands Lp.

Preferably M is a metal ion having an unfilled inner shell and the preferred metals are selected from Sm(III), Eu(II), Eu(III), Tb(III), Dy(III), Yb(III), Lu(III), Gd (III), Gd(III) U(III), Tm(III), Ce (III), Pr(III), Nd(III), Pm(III), Dy(III), Ho(III), Er(III) and more preferably Eu(III), Tb(III), Dy(III), Gd (III).

Further compounds which can be used in the present invention are of general formula $(L\alpha)_nM_1M_2$ where M_1 is the same as M above, M_2 is a non rare earth metal, $L\alpha$ is as above and n is the combined valence state of M_1 and M_2 . The complex can also comprise one or more neutral ligands Lp so the complex has the general formula $(L\alpha)_n M_1 M_2$ (Lp), where Lp is as above. The metal M_2 can be any metal which is not a rare earth, transition metal, lanthanide or an actinide; examples of metals which can be used include lithium, sodium, potassium, rubidium, caesium, beryllium, magnesium, calcium, strontium, barium, copper (I), copper (II), silver, gold, zinc, cadmium, boron, aluminium, gallium, indium, germanium, tin (II), tin (IV), antimony (II), antimony (IV), lead (IV) and metals of the first, second and third groups of transition metals in different valence states e.g. manganese, iron, ruthenium, osmium, cobalt, nickel, palladium(II), palladium(IV), platinum(II), platinum(IV), cadmium, chromium. titanium, vanadium, zirconium, tantulum, molybdenum, rhodium, iridium, titanium, niobium, scandium, yttrium.

For example $(L_1)(L_2)(L_3)(L..)M$ (Lp) where M is a rare earth, transition metal, lanthanide or an actinide and $(L_1)(L_2)(L_3)(L...)$ and (Lp) are the same or different organic complexes.

Further organometallic complexes which can be used in the present invention are binuclear, trinuclear and polynuclear organometallic complexes e.g. of formula

30 $(Lm)_x M_1 \leftarrow M_2(Ln)_y$ e.g.

$$(Lm)_x M_1 \stackrel{L}{\sim} M_2 (Ln)_y$$

where L is a bridging ligand and where M_1 is a rare earth metal and M_2 is M_1 or a non rare earth metal, Lm and Ln are the same or different organic ligands $L\alpha$ as defined above, x is the valence state of M_1 and y is the valence state of M_2 .

In these complexes there can be a metal to metal bond or there can be one or more bridging ligands between M_1 and M_2 and the groups Lm and Ln can be the same or different.

By trinuclear is meant there are three rare earth metals joined by a metal to metal bond i.e. of formula

$$(Lm)_x M_1 \longrightarrow M_3 (Ln)_y \longrightarrow M_2 (Lp)_z$$

or

15

25

5

10

$$(Lm)_x M_1 \longrightarrow M_3 (Ln)_y$$
 M_2
 $(Lp)_z$

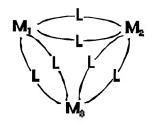
where M_1 , M_2 and M_3 are the same or different rare earth metals and Lm, Ln and Lp are organic ligands, L α and x is the valence state of M_1 , y is the valence state of M_2 and z is the valence state of M_3 . Lp can be the same as Lm and Ln or different.

The rare earth metals and the non rare earth metals can be joined together by a metal to metal bond and/or via an intermediate bridging atom, ligand or molecular group.

For example the metals can be linked by bridging ligands e.g.

$$(Lm)_x M_1 M_3 (Ln)_y M_2 (Lp)_z$$

5 or



where L is a bridging ligand

By polynuclear is meant there are more than three metals joined by metal to metal bonds and/or via intermediate ligands

$$M_1 - M_2 - M_3 - M_4$$

or

15

$$M_1 - M_2 - M_4 - M_3$$

or

20 or

- 8 -

5

10

20

where M₁, M₂, M₃ and M₄ are rare earth metals and L is a bridging ligand.

The metal M_2 can be any metal which is not a rare earth, transition metal, lanthanide or an actinide examples of metals which can be used include lithium, sodium, potassium, rubidium, caesium, beryllium, magnesium, calcium, strontium, barium, copper, silver, gold, zinc, cadmium, boron, aluminium, gallium, indium, germanium, tin, antimony, lead, and metals of the first, second and third groups of transition metals e.g. manganese, iron, ruthenium, osmium, cobalt, nickel, palladium, platinum, cadmium, chromium. titanium, vanadium, zirconium, tantulum, molybdenum, rhodium, iridium, titanium, niobium, scandium, yttrium etc.

Preferably L α is selected from β diketones such as those of formulae

$$\begin{pmatrix}
R_1 \\
R_2 \\
R_3
\end{pmatrix}$$
or
$$\begin{pmatrix}
R_1 \\
R_2 \\
R_3
\end{pmatrix}$$
or
$$\begin{pmatrix}
R_1 \\
R_2 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_2 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_2 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_2 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_3 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_2 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_3 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_2 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_3 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_2 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_3 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_2 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_2 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_2
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_3
\end{pmatrix}$$

where R₁, R₂ and R₃ can be the same or different and are selected from hydrogen, and substituted and unsubstituted hydrocarbyl groups such as substituted and unsubstituted aliphatic groups, substituted and unsubstituted aromatic, heterocyclic and polycyclic ring structures, fluorocarbons such as trifluoryl methyl groups, halogens such as fluorine or thiophenyl groups; R₁, R₂ and R₃ can also form substituted and unsubstituted fused aromatic, heterocyclic and polycyclic ring structures and can be copolymerisable with a monomer e.g. styrene. X is Se, S or O, Y can be hydrogen, substituted or unsubstituted hydrocarbyl groups, such as substituted and unsubstituted aromatic, heterocyclic and polycyclic ring structures,

- 9 -

fluorine, fluorocarbons such as trifluoryl methyl groups, halogens such as fluorine or thiophenyl groups or nitrile.

Examples of R₁ and/or R₂ and/or R₃ include aliphatic, aromatic and heterocyclic alkoxy, aryloxy and carboxy groups, substituted and substituted phenyl, fluorophenyl, biphenyl, phenanthrene, anthracene, naphthyl and fluorene groups alkyl groups such as t-butyl, heterocyclic groups such as carbazole.

Some of the different groups $L\alpha$ may also be the same or different charged groups such as carboxylate groups so that the group L_1 can be as defined above and the groups L_2 , L_3 ... can be charged groups such as

$$R - C$$
 C
 C
 C
 C
 C

where R is R_1 as defined above or the groups L_1 , L_2 can be as defined above and $L_{3...}$ etc. are other charged groups.

R₁, R₂ and R₃ can also be

5

15

A preferred moiety R₁ is trifluoromethyl CF₃ and examples of such diketones are, banzoyltrifluoroacetone, p-chlorobenzoyltrifluoroacetone, p-bromotrifluoroacetone, p-phenyltrifluoroacetone, 1-naphthoyltrifluoroacetone, 2-naphthoyltrifluoroacetone, 2-phenathoyltrifluoroacetone, 3-phenanthoyltrifluoroacetone, 9-anthroyltrifluoroacetonetrifluoroacetone, cinnamoyltrifluoroacetone, and 2-thenoyltrifluoroacetone.

5

The different groups $L\alpha$ may be the same or different ligands of formulae

$$\begin{pmatrix}
R_1 & X & X \\
R_3 & X & X \\
R_2 & X & X
\end{pmatrix}$$
(VI)

where X is O, S, or Se and R₁ R₂ and R₃ are as above.

The different groups La may be the same or different quinolate derivatives such as

where R is hydrocarbyl, aliphatic, aromatic or heterocyclic carboxy, aryloxy, hydroxy or alkoxy e.g. the 8 hydroxy quinolate derivatives or

$$R \longrightarrow B \longrightarrow O^{-} \qquad R_{1} \longrightarrow O^{-} \qquad O^{-} \longrightarrow O^{-} \qquad O^{-} \longrightarrow O^{-$$

where R, R_1 , and R_2 are as above or are H or F e.g. R_1 and R_2 are alkyl or alkoxy groups

$$\begin{array}{c} CF_3 \\ S \\ O \\ CF_3 \\ O \\ CF_3 \\ O \end{array}$$

As stated above the different groups $L\alpha$ may also be the same or different carboxylate groups e.g.

where R_5 is a substituted or unsubstituted aromatic, polycyclic or heterocyclic ring a polypyridyl group, R_5 can also be a 2-ethyl hexyl group so L_n is 2-ethylhexanoate or R_5 can be a chair structure so that L_n is 2-acetyl cyclohexanoate or $L\alpha$ can be

$$CF_3$$
 CIV
 CIV
 CIV

where R is as above e.g. alkyl, allenyl, amino or a fused ring such as a cyclic or polycyclic ring.

5 The different groups Lα may also be

$$\begin{pmatrix}
R_1 \\
R_2 \\
N \\
-X
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 \\
R_2
\end{pmatrix}$$
or
$$\begin{pmatrix}
R_1 \\
R_2
\end{pmatrix}$$
or
$$\begin{pmatrix}
XVI
\end{pmatrix}$$

10

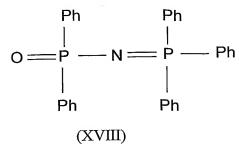
$$R_3$$
 R_1
 R_2
 R_3
 R_1
 R_2
 R_2
 R_3
 R_2
 R_3
 R_2
 R_3
 R_2
 R_3
 R_2
 R_3
 R_4
 R_2

Where R, R_1 and R_2 are as above.

15

The groups L_P can be selected from

- 13 -



where each Ph which can be the same or different and can be a phenyl (OPNP) or a substituted phenyl group, other substituted or unsubstituted aromatic group, a substituted or unsubstituted heterocyclic or polycyclic group, a substituted or unsubstituted fused aromatic group such as a naphthyl, anthracene, phenanthrene or pyrene group. The substituents can be for example an alkyl, aralkyl, alkoxy, aromatic, heterocyclic, polycyclic group, halogen such as fluorine, cyano, amino. Substituted amino etc. Examples are given in figs. 1 and 2 of the drawings where R, R₁, R₂, R₃ and R₄ can be the same or different and are selected from hydrogen, hydrocarbyl groups, substituted and unsubstituted aromatic, heterocyclic and polycyclic ring structures, fluorocarbons such as trifluoryl methyl groups, halogens such as fluorine or thiophenyl groups; R, R₁, R₂, R₃ and R₄ can also form substituted and unsubstituted fused aromatic, heterocyclic and polycyclic ring structures and can be copolymerisable with a monomer e.g. styrene. R, R₁, R₂, R₃ and R₄ can also be unsaturated alkylene groups such as vinyl groups or groups

$$---$$
C $---$ CH $_2$ $---$ CH $_2$ $---$ R

where R is as above.

20

5

10

15

L_p can also be compounds of formulae

- 14 -

$$R_1$$
 R_2
 R_1
 R_2
 R_3
 R_4
 R_5
 R_7
 R_8
 R_8
 R_8
 R_8
 R_8
 R_8
 R_9
 R_9

where R_1 , R_2 and R_3 are as referred to above, for example bathophen shown in fig. 3 of the drawings in which R is as above or

5

where R_1 , R_2 and R_3 are as referred to above.

10

L_p can also be

$$S \stackrel{Ph}{=} \stackrel{Ph}{=}$$

where Ph is as above.

Other examples of L_p chelates are as shown in figs. 4 and fluorene and fluorene derivatives e.g. a shown in figs. 5 and compounds of formulae as shown as shown in figs. 6 to 8.

Specific examples of L α and Lp are tripyridyl and TMHD, and TMHD complexes, α , α ', α " tripyridyl, crown ethers, cyclans, cryptans phthalocyanans, porphoryins ethylene diamine tetramine (EDTA), DCTA, DTPA and TTHA, where TMHD is 2,2,6,6-tetramethyl-3,5-heptanedionato and OPNP is diphenylphosphonimide triphenyl phosphorane. The formulae of the polyamines are shown in fig. 9.

10

15

20

25

30

Other electroluminescent materials which can be used include metal quinolates such as lithium quinolate, aluminium quinolate, scandium quinolate zirconium quinolate, hafnium quinolate vanadium quinolate etc. The quinolates can be doped e.g. with a dye such as diphenylquinacridine, diphenylquinacridone, coumarins, perylene and their derivatives.

Other electroluminescent materials which can be used include organic complexes of non rare earth metals such as lithium, sodium, potassium, rubidium, caesium, beryllium, magnesium, calcium, strontium, barium, copper, silver, gold, zinc, cadmium, boron, aluminium, gallium, indium, germanium, tin, antimony, lead, and metals of the first, second and third groups of transition metals e.g. manganese, iron, ruthenium, osmium, cobalt, nickel, palladium, platinum, cadmium, chromium. titanium, vanadium, zirconium, tantulum, molybdenum, rhodium, iridium, titanium, niobium, scandium, yttrium etc. which emit light when an electric current is passed through it. The complexes can be formed with the ligands of formula (I) to (XVII)

Such complexes are complexes of β -diketones e.g. tris -(1,3-diphenyl-1-3-propanedione) (DBM) and suitable metal complexes are Al(DBM)₃, Zn(DBM)₂ and Mg(DBM)₂... Sc(DBM)₃ etc.

above, optionally with a neutral ligand of formula L_p as defined above.

Further complexes which can be used as the photovoltaic element are borate complexes of formula

$$R_1$$
 R_2
 R_3

where M is a rare earth, lanthanide or an actinide and R_{1} , R_{2} and R_{3} are as defined above.

A photovoltaic device can be made in the conventional way for example by forming a layer of the metal chelate on a metal so the metal forms a first electrode and preferably the other, second electrode, comprises a transparent conductive layer. This electrode is preferably a transparent substrate which is a conductive glass or plastic material which acts as the cathode; preferred substrates are conductive glasses such as indium tin oxide coated glass, but any glass which is conductive or has a conductive layer can be used, so that, when light falls on the metal chelate an electric field is generated between the electrodes.

15

10

5

There are a very large number of designs for photovoltaic devices and solar cells and a survey of such devices is given in the Jean-Michel Nunzi Article referred to above and in the references thereto. In general the metal chelates can be used as the photovoltaic element in such devices.

- 17 -

The metal chelate material can be deposited on the metal or conductive transparent material substrate directly by evaporation from a solution of the material in an organic solvent. The solvent which is used will depend on the material, but chlorinated hydrocarbons such as dichloromethane, n-methyl pyrrolidone, dimethyl sulphoxide, tetra hydrofuran dimethylformamide etc. are suitable in many cases.

Alternatively the material can be deposited by spin coating from solution or by vacuum deposition from the solid state e.g. by sputtering or any other conventional method can be used.

As stated above, the electrons by absorption of solar radiation of the appropriate bandgap, produce electron-hole pairs. The separation of the electron-hole pairs with the electrons flowing toward the region of N-type conductivity, and the holes flowing toward the region of P-type conductivity, creates the photovoltage and photocurrent of the cell. By having a layer of a hole transmitting material, i.e. a p-type transmitter between the cathode and the metal chelate and/or a layer of an electron transmitting material between the metal chelate and the anode, increased mobility of the holes and the electrons can be achieved increasing the effectiveness of the photovoltaic cell.

20

25

5

10

15

Hole transmitting layers are used in polymer electroluminescent devices and any of the known hole transmitting materials in film form can be used.

The hole transporting material can be an amine complex such as poly (vinylcarbazole), N, N'-diphenyl-N, N'-bis (3-methylphenyl) -1,1' -biphenyl -4,4'-diamine (TPD), an unsubstituted or substituted polymer of an amino substituted aromatic compound, a polyaniline, substituted polyanilines, polythiophenes, substituted polythiophenes, polysilanes etc. Examples of polyanilines are polymers of

- 18 -

5 where R is in the ortho – or meta-position and is hydrogen, C1-18 alkyl, C1-6 alkoxy, amino, chloro, bromo, hydroxy or the group

where R is alky or aryl and R' is hydrogen, C1-6 alkyl or aryl with at least one other monomer of formula I above.

Or the hole transporting material can be a polyaniline. Polyanilines which can be used in the present invention have the general formula

$$\begin{array}{c|c}
 & R \\
 & R \\$$

15

20

where p is from 1 to 10 and n is from 1 to 20, R is as defined above and X is an anion, preferably selected from Cl, Br, SO₄, BF₄, PF₆, H₂PO₃, H₂PO₄, arylsulphonate, arenedicarboxylate, polystyrenesulphonate, polyacrylate alkysulphonate, vinylsulphonate, vinylbenzene sulphonate, cellulose sulphonate, camphor sulphonates, cellulose sulphate or a perfluorinated polyanion.

Examples of arylsulphonates are p-toluenesulphonate, benzenesulphonate, 9,10-anthraquinone-sulphonate and anthracenesulphonate; an example of an arenedicarboxylate is phthalate and an example of arenecarboxylate is benzoate.

5

10

15

25

We have found that protonated polymers of the unsubstituted or substituted polymer of an amino substituted aromatic compound such as a polyaniline are difficult to evaporate or cannot be evaporated, however we have surprisingly found that if the unsubstituted or substituted polymer of an amino substituted aromatic compound is deprotonated then it can be easily evaporated i.e. the polymer is evaporable.

Preferably evaporable deprotonated polymers of unsubstituted or substituted polymer of an amino substituted aromatic compound are used. The de-protonated unsubstituted or substituted polymer of an amino substituted aromatic compound can be formed by deprotonating the polymer by treatment with an alkali such as ammonium hydroxide or an alkali metal hydroxide such as sodium hydroxide or potassium hydroxide.

The degree of protonation can be controlled by forming a protonated polyaniline and de-protonating. Methods of preparing polyanilines are described in the article by A. G. MacDiarmid and A. F. Epstein, Faraday Discussions, Chem Soc.88 P319 1989.

The conductivity of the polyaniline is dependant on the degree of protonation with the maximum conductivity being when the degree of protonation is between 40 and 60% e.g. about 50%.

Preferably the polymer is substantially fully deprotonated.

A polyaniline can be formed of octamer units i.e. p is four e.g.

The polyanilines can have conductivities of the order of 1 x 10⁻¹ Siemen cm⁻¹ or higher.

5

The aromatic rings can be unsubstituted or substituted e.g. by a C1 to 20 alkyl group such as ethyl.

The polyaniline can be a copolymer of aniline and preferred copolymers are the copolymers of aniline with o-anisidine, m-sulphanilic acid or o-aminophenol, or o-toluidine with o-aminophenol, o-ethylaniline, o-phenylene diamine or with amino anthracenes.

Other polymers of an amino substituted aromatic compound which can be used include substituted or unsubstituted polyaminonapthalenes, polyaminoanthracenes, polyaminophenanthrenes, etc. and polymers of any other condensed polyaromatic compound. Polyaminoanthracenes and methods of making them are disclosed in US Patent 6,153,726. The aromatic rings can be unsubstituted or substituted e.g. by a group R as defined above.

20

Other hole transporting materials are conjugated polymer and the conjugated polymers which can be used can be any of the conjugated polymers disclosed or referred to in US 5807627, PCT/WO90/13148 and PCT/WO92/03490.

25 The preferred conjugated polymers are poly (p-phenylenevinylene)-PPV and copolymers including PPV. Other preferred polymers are poly(2,5 dialkoxyphenylene vinylene) such as poly (2-methoxy-5-(2-methoxypentyloxy-1,4-phenylene vinylene), poly(2-methoxypentyloxy)-1,4-phenylenevinylene), poly(2-methoxy-5-(2-dodecyloxy-1,4-phenylenevinylene) and other poly(2,5 dialkoxyphenylenevinylenes)

- 21 -

with at least one of the alkoxy groups being a long chain solubilising alkoxy group, polyfluorenes and oligofluorenes, polyphenylenes and oligophenylenes, polyanthracenes and oligo anthracenes, ploythiophenes and oligothiophenes.

In PPV the phenylene ring may optionally carry one or more substituents e.g. each independently selected from alkyl, preferably methyl, alkoxy, preferably methoxy or ethoxy.

Any poly(arylenevinylene) including substituted derivatives thereof can be used and the phenylene ring in poly(p-phenylenevinylene) may be replaced by a fused ring system such as anthracene or naphthlyene ring and the number of vinylene groups in each polyphenylenevinylene moiety can be increased e.g. up to 7 or higher.

The conjugated polymers can be made by the methods disclosed in US 5807627, PCT/WO90/13148 and PCT/WO92/03490.

The thickness of the hole transporting layer is preferably 20nm to 200nm.

15

25

30

The polymers of an amino substituted aromatic compound such as polyanilines referred to above can also be used as buffer layers with or in conjunction with other hole transporting materials.

The structural formulae of some other hole transporting materials are shown in Figures 12, 13, 14, 15 and 16 of the drawings, where R_1 , R_2 and R_3 can be the same or different and are selected from hydrogen, and substituted and unsubstituted hydrocarbyl groups such as substituted and unsubstituted aliphatic groups, substituted and unsubstituted aromatic, heterocyclic and polycyclic ring structures, fluorocarbons such as trifluoryl methyl groups, halogens such as fluorine or thiophenyl groups; R_1 , R_2 and R_3 can also form substituted and unsubstituted fused aromatic, heterocyclic and polycyclic ring structures and can be copolymerisable with a monomer e.g.

- 22 -

PCT/GB2003/003035

styrene. X is Se, S or O, Y can be hydrogen, substituted or unsubstituted hydrocarbyl groups, such as substituted and unsubstituted aromatic, heterocyclic and polycyclic ring structures, fluorine, fluorocarbons such as trifluoryl methyl groups, halogens such as fluorine or thiophenyl groups or nitrile.

5

WO 2004/008554

Examples of R₁ and/or R₂ and/or R₃ include aliphatic, aromatic and heterocyclic alkoxy, aryloxy and carboxy groups, substituted and substituted phenyl, fluorophenyl, biphenyl, phenanthrene, anthracene, naphthyl and fluorene groups alkyl groups such as t-butyl, heterocyclic groups such as carbazole.

10

15

Optionally there is a layer of an electron injecting material between the anode and the electroluminescent material layer; the electron injecting material is a material which will transport electrons when an electric current is passed through it; electron injecting materials include a metal complex such as a metal quinolate e.g. an aluminium quinolate, lithium quinolate, a cyano anthracene such as 9,10 dicyano anthracene, cyano substituted aromatic compounds, tetracyanoquinidodimethane a polystyrene sulphonate or a compound with the structural formulae shown in figures 9 or 10 of the drawings in which the phenyl rings can be substituted with substituents R as defined above.

20

The cathode is preferably a transparent substrate such as a conductive glass or plastic material which acts as the anode. Preferred substrates are conductive glasses such as indium tin oxide coated glass, but any glass which is conductive or has a conductive layer such as a metal or conductive polymer can be used. Conductive polymers and conductive polymer coated glass or plastics materials can also be used as the substrate.

25

The anode is preferably a low work function metal e.g. aluminium, calcium, lithium, silver/magnesium alloys, rare earth metal alloys etc., aluminium is a preferred metal.

A metal fluoride such as an alkali metal, rare earth metal or their alloys can be used as the second electrode for example by having a metal fluoride layer formed on a metal.

- As stated above, the photocurrent output of a solar cell is maximized by increasing the total number of photons of differing energy and wavelength which are absorbed by the semiconductor material and it is a feature of the present invention that the rare earth metal chelates can absorb light of a specific wavelength depending on the metal and ligands used so, by having a plurality of layers of different metal chelates of differing bandgaps which absorb light at different wavelengths, a wide range of the visible spectrum can be used. Metal chelates can be also used which will absorb light in the infra-red, ultra-violet or shorter wavelengths so improving the utilisation of sunlight and increasing the power achievable by a solar cell.
- As stated above, the photocurrent output of a solar cell is maximized by increasing the total number of photons of differing energy and wavelength which are absorbed by the semiconductor material and it is a feature of the present invention that the rare earth metal chelates can absorb light of a specific wavelength depending on the metal and ligands used so, by having a plurality of layers of different metal chelates of differing bandgaps which absorb light at different wavelengths, a wide range of the visible spectrum can be used. Metal chelates can be also used which will absorb light in the infra-red, ultra-violet or shorter wavelengths so improving the utilisation of sunlight and increasing the power achievable by a solar cell.
- Alternatively individual solar cells of differing bandgap energies i.e. using different metal chelates of differing bandgaps which absorb light at different wavelengths can be connected in series.

Devices of the invention are illustrated in the drawings in which:-

- 24 -

Fig. 17 shows a simple photovoltaic cell

Figs. 18 and 19 show other cells and

Fig. 20 shows a tandem cell

5

10

Referring to fig. 17 a simple cell comprises a metal anode e.g. made of aluminium (1) a layer of an electroluminescent material (2) as described herein and a cathode comprising an indium titanium oxide (ITO) coated glass (3). When light passes through the ITO coated glass it is absorbed by the electroluminescent material layer (2), which is the photovoltaic element, and an electric field is generated between the anode and cathode and when the anode and cathode are connected through an electric circuit an electric current will flow between them.

Referring to fig. 18 there is a layer of an electron transmitting material (4) between the layers (2) and (1).

Referring to fig. 19 there is a layer of a hole transporting layer (5) between the layers (2) and (3).

20 Referring to fig. 20 this shows a tandem solar cell in which there are a plurality of cells in series of fig. 17 formed of a cathode (11), an electroluminescent layer (13) and anode (12) so that a larger field is generated between the end anode and cathode, in order for there to be a transmission of light through the cells the anodes and cathodes of the intermediate cells are transparent. At least some of the photovoltaic elements (13) in each of the cells are different to adsorb light at a range of wavelengths.

Example 1

30

A photovoltaic device was fabricated on a clean and dried ITO coated glass piece (1 x 1cm²) by sequentially forming layers by vacuum evaporation to form a structure

PCT/GB2003/003035

ITO/CuPc(20nm)/TPD(50nm)/ Eu (DBM)₃(OPNP)/(85nm)Alq₃/LiF(0.4nm)/Al

Where CuPc is copper phthalocyanine, TPD is N, N'-diphenyl-N, N'-bis (3-methylphenyl) -1,1' -biphenyl -4,4'-diamine, Alq₃ is aluminium quinolate, LiF is lithium fluoride and Al is aluminium.

To deposit the layers the organic coating on the portion which had been etched with the concentrated hydrochloric acid was wiped with a cotton bud. The coated electrodes were stored in a vacuum desiccator over a molecular sieve and phosphorous pentoxide until they were loaded into a vacuum coater (Edwards, 10^{-6} torr) and aluminium top contacts made. The active area of the photovoltaic device was 0.08 cm by 0.1 cm² the devices were then kept in a vacuum desiccator until the photovoltaic studies were performed.

15

20

10

5

The device was connected in an electric circuit and exposed to light of various wavelengths λ and the voltage and current measured the results are shown graphically in fig. 21 where the open circuit voltage Voc and short circuit current Jsc (as described in the Jean-Michel Nunzi Article referred to above) were obtained. The white light was obtained from a simulated daylight fluorescent bulb.

Example 2

Example 1 was repeated using a structure comprising

25

ITO/CuPc(20nm)/α-NPB(75nm)/Zrq₄:DPQA(75:0.75nm)/Zrq₄10nm)Alq₃/LiF(0.4nm/Al

Where α -NPB is as shown in fig. 16a, DPQA is diphenylquinacridone.

The Zrq₄ is zirconium quinolate and the Zrq₄:DPQA layer was formed by concurrent vacuum deposition to form a zirconium quinolate layer doped with DPQA. The weight ratio of the Zrq₄ and DPQA is conveniently shown by a relative thickness measurement.

5

The device was connected in an electric circuit and exposed to light of various wavelengths λ and the voltage and current measured the results are shown graphically in fig. 22 where the open circuit voltage Voc and short circuit current Jsc (as described in the Jean-Michel Nunzi Article referred to above) were obtained. The white light was obtained from a simulated daylight fluorescent bulb.

Example 3

Example 1 was repeated using a structure comprising

15

10

ITO/CuPc(20nm)/α-NPB(75nm)/Liq(65nm/Al.

Where Liq is lithium quinolate

The device was connected in an electric circuit and exposed to light of various wavelengths λ and the voltage and current measured the results are shown graphically in fig. 23 where the open circuit voltage Voc and short circuit current Jsc (as described in the Jean-Michel Nunzi Article referred to above) were obtained. The white light was obtained from a simulated daylight fluorescent bulb.

25

Example 4

Example 1 was repeated using a structure comprising

 $ITO/CuPc(20nm)/\alpha-NPB(75nm)/Liq(65nm)LiF(0.4nm/A1.$

The device was connected in an electric circuit and exposed to light of various wavelengths λ and the voltage and current measured the results are shown graphically in fig. 24 where the open circuit voltage Voc and short circuit current Jsc (as described in the Jean-Michel Nunzi Article referred to above) were obtained. The white light was obtained from a simulated daylight fluorescent bulb.

Example 5

10

5

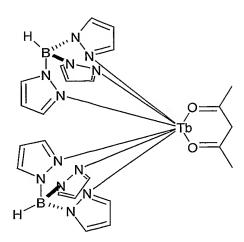
Devices were made as in Example 1 of structure $ITO/CuPc(25)/\alpha-NPB(80)/CBP:Compound\ A(30:2)/BCP(10)/Zrq_4(60)/LiF(0.2)/Al$

Where the film thicknesses are in nanometres and CBP is as in fig. 4b and BCP is bathocupron

compound A was

Similar devices were made with compounds B and C in place of compound A where compound B is

- 28 -



and compound C is

5

The results are shown in the Table

Table

Photovoltaic element	V ^{OC} _{Ph} / mV	J ^{SC} _{Ph} / mA cm ⁻²	λ/nm
A	7.5	- 0.4	600
В	-0.3	2.2	500
С	-159	0.4	550

Claims

1. A photovoltaic device comprising a metal chelate as the photovoltaic element.

- 29 -

- 2. A photovoltaic device as claimed in claim 1 which comprises sequentially (i) a first electrode comprising a metal, (ii) the photovoltaic element and (iii) a second electrode.
- 3. A device as claimed in claim 1 or 2 in which the photovoltaic element comprises an organo metallic complex of formula

$$(L\alpha)_nM$$
 or $(L\alpha)_n > M \leftarrow Lp$

where Lα and Lp are organic ligands, M is a metal and n is the valence state of the metal M and in which the ligands Lα are the same or different.

- 4. A device as claimed in any one of claims 1 to 4 in which the metal M is a rare earth, transition metal, lanthanide or an actinide.
- 5. A device as claimed in claim 4 in which the said rare earth, transition metal, lanthanide or an actinide is selected from Sm(III), Eu(II), Eu(III), Tb(III), Dy(III), Yb(III), Lu(III), Gd (III), Gd(III) U(III), Tm(III), Ce (III), Pr(III), Nd(III), Pm(III), Dy(III), Ho(III) and Er(III).
- 6. A device as claimed in any one of claims 1 to 3 in which the metal M is a non rare earth metal.
 - 7. A device as claimed in claim 6 in which the metal M is selected from lithium, sodium, potassium, rubidium, caesium, beryllium, magnesium, calcium, strontium,

barium, copper, silver, gold, zinc, cadmium, boron, aluminium, gallium, indium, germanium, tin, antimony, lead, and metals of the first, second and third groups of transition metals, manganese, iron, ruthenium, osmium, cobalt, nickel, palladium, platinum, cadmium, chromium. titanium, vanadium, zirconium, tantulum, molybdenum, rhodium, iridium, titanium, niobium, scandium and yttrium.

- 8. A device as claimed in any one of claims 3 to 7 in which there are a plurality of ligands Lp which can be the same or different.
- 9. A device as claimed in any one of the preceding claims in which the photovoltaic element comprises an organo metallic complex of formula $(L_n)_n M_1 M_2$ or $(L_n)_n M_1 M_2$ (L_p) , where L_n is $L\alpha$, L_p is a neutral ligand M_1 is a rare earth, transition metal, lanthanide or an actinide, M_2 is a non rare earth metal and n is the combined valence state of M_1 and M_2 .

15

5

10. A device as claimed in any one of the preceding claims in which the photovoltaic element comprises a binuclear, trinuclear or polynuclear organometallic complex of formula

$$(Lm)_x M_1 \leftarrow M_2(Ln)_y$$
 or

$$(Lm)_x M_1 \stackrel{L}{\searrow} M_2 (Ln)_y$$

20

where L is a bridging ligand and where M_1 is a rare earth metal and M_2 is M_1 or a non rare earth metal, Lm and Ln are the same or different organic ligands L α as defined above, x is the valence state of M_1 and y is the valence state of M_2 or

$$(Lm)_x M_1 - M_3 (Ln)_y - M_2 (Lp)_z$$

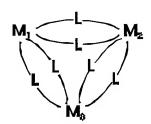
- 31 -

$$(Lm)_x M_1 \longrightarrow M_3 (Ln)_y$$
 M_2
 $(Lp)_z$

where M_1 , M_2 and M_3 are the same or different rare earth metals and Lm, Ln and Lp are organic ligands $L\alpha$ and x is the valence state of M_1 , y is the valence state of M_2 and z is the valence state of M_3 and Lp can be the same as Lm and Ln or different or

$$(Lm)_x M_1 M_3 (Ln)_y M_2 (Lp)_z$$

10 or



or

or

15
$$M_1 - M_2 - M_3 - M_4$$

$$M_1 \longrightarrow M_2 \longrightarrow M_4 \longrightarrow M_3$$

20

or

where M₄ is M₁ and L is a bridging ligand and in which the rare earth metals and the non rare earth metals can be joined together by a metal to metal bond and/or via an intermediate bridging atom, ligand or molecular group or in which there are more than three metals joined by metal to metal bonds and/or via intermediate ligands and

- 10 11. A device as claimed in any one of claims 3 to 10 in which $L\alpha$ has the formula (I) to (XVII) herein.
 - 12. A device as claimed in any one of claims 3 to 11 in which Lp has the formula of figs. 1 to 8 of the accompanying drawings or of formula (XVIII) to (XXV) herein.

13. A device as claimed in claim 1 or 2 in which the organometallic chelate is a metal quinolate.

- 14. A device as claimed in claim 13 in which the metal quinolate is lithium quinolate, aluminium quinolate, scandium quinolate zirconium quinolate, hafnium quinolate or vanadium quinolate.
 - 15. A device as claimed in claim 14 in which the metal quinolate is doped with a fluorescent, phosphorescence or ion fluorescent compound.

15

20

- 33 -

16. A device as claimed in claim 15 in which the dopant is diphenylquinacridine, diphenylquinacridone, coumarins, perylene or their derivatives.

17. A device as claimed in claim 1 or 2 in which the photovoltaic element has the formula

$$R_1$$
 R_2
 R_3

5

where M is a rare earth, transition metal, lanthanide or an actinide and R₁, R₂ and R₃

can be the same or different and are selected from hydrogen, and substituted and unsubstituted hydrocarbyl groups, substituted and unsubstituted aliphatic groups, substituted and unsubstituted aromatic, heterocyclic and polycyclic ring structures, fluorocarbons and trifluoryl methyl groups, halogens and thiophenyl groups.

18. A device as claimed in any one of claims 2 to 17 in which the second electrode comprises a transparent substrate which is a conductive glass or plastic material and which covers at least part of the pholtovoltaic element.

- 34 -

19. A device as claimed in any one of the preceding claims which comprises sequentially (i) a first electrode comprising a metal, (ii) a plurality of layers of photovoltaic elements in which the photovoltaic elements in at least two of the layers are different and (iii) a second electrode.

5

20. A device as claimed in claim 19 in which at least some of the different photovoltaic elements absorb light at different wavelengths.

$$\begin{array}{c|c}
R_1 & R_2 \\
\hline
O = P - N = P \\
\hline
R_3 & R_4
\end{array}$$

$$O = \begin{array}{c|c} Ph & Ph \\ \hline P & Ph \\ \hline P & P \\ \hline P & P \\ \hline Ph & Ph \\ \hline Ph & Ph \\ \hline NR_1R_2 \\ \hline NR_1R_2 \\ \hline \end{array}$$

Fig. 2b

Fig. 3

2/24

Fig. 4c

Fig. 4g

$$\begin{array}{c} R \\ R \\ N \\ \end{array}$$

Fig. 4d

Fig. 4e

N N N N

Fig. 4h

Fig. 4j

Fig.4k

Fig. 4l

$$R_4$$
 P
 R_2
 R_1
 R_2

Fig.5b

Fig. 5d

Fig. 6e

$$R$$
 R_2N
 R_2N

Fig 5f

Fig 6b

$$R_1$$

Fig. 6d

R
$$(CH_2)_n$$
 $S = 0$

R
 $m = 0,1,2 \text{ etc.}$
 $n = 0,1,2 \text{ etc.}$

Fig. 7c

Fig. 7b

$$\begin{pmatrix}
R_2 & R_1 \\
R_3 & N \\
R_1 & P = N
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 & P \\
R_2 & N \\
R_3 & N \\
R_1 & N \\
R_2 & R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 & N \\
R_2 & R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 & N \\
R_2 & R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 & N \\
R_2 & R_3
\end{pmatrix}$$

$$\begin{pmatrix}
R_1 & N \\
R_2 & R_3
\end{pmatrix}$$

Fig. 7d

$$R'$$
 $S = 0$
 $(CH_2)_n$
 R
 $n = 0,1,2 \text{ etc.}$

$$CH_2$$
 $\rightarrow R$
 $S = O$
 $(CH_2)_m$
 $m = 0,1,2 \text{ etc.}$
 $m = 0,1,2 \text{ etc.}$

Fig. 7f

$$R_1$$
 R_2 R_2 R_3 R_4 R_5 R_5

Fig. 8b

Fig. 8c

Fig.8d

Fig. 8e

O

$$CH_2$$
 $\int_{n}^{0} S - (CH_2)_{m} - R$
 $M = 0,1,2 \text{ etc.}$
 $n = 0,1,2 \text{ etc.}$

Fig. 8f

$$R$$
 R
 CH_2
 R
 CH_2
 R

Fig. 8g

Fig. 8h

$$H_3C$$
 CH_3
 CH_3

Fig. 9

OXD- Star

Fig. 10

11/24

$$H_2NH_2C$$
 N
 CH_2NH_2
 CH_2NH_2
 CH_2NH_2

EDTA

$$CH_2NH_2$$
 CH_2NH_2
 CH_2NH_2
 CH_2NH_2
 CH_2NH_2
 CH_2NH_2

TTHA

Fig. 11

Fig. 12d

Fig. 13c

$$R_1$$
 R_2
 R_3
 R_4
 R_1
 R_2
Fig. 14a
Fig. 14b

$$R_1$$
 R_2
 S
 R_3
 R_4
or

$$R_1$$
 S
 S
 S
 S
 R_3
 R_4

Fig. 14c

Fig. 14d

Fig. 15a

Fig. 15b

16/24

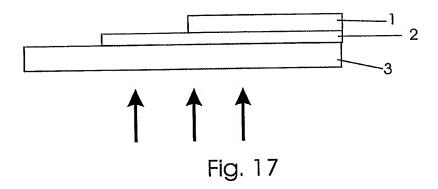
$$\alpha$$
 -NPB

Fig. 16a

Fig. 16b

mTADATA

Fig. 16c



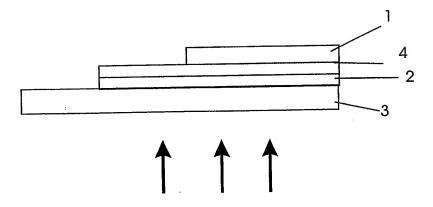
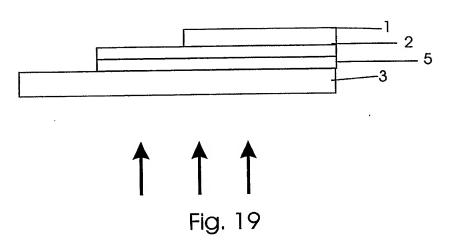


Fig. 18



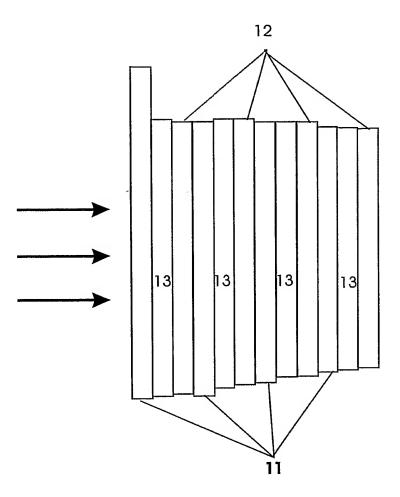


Fig. 20

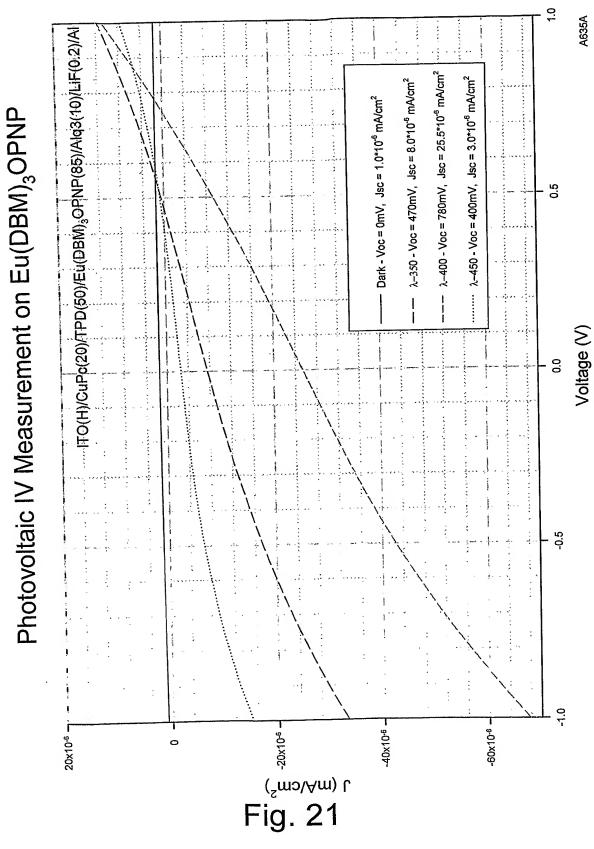
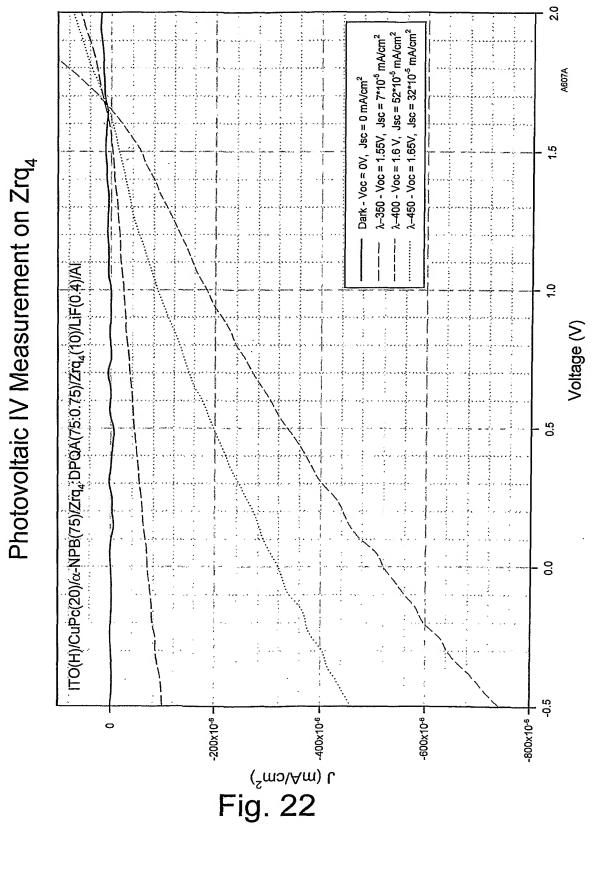
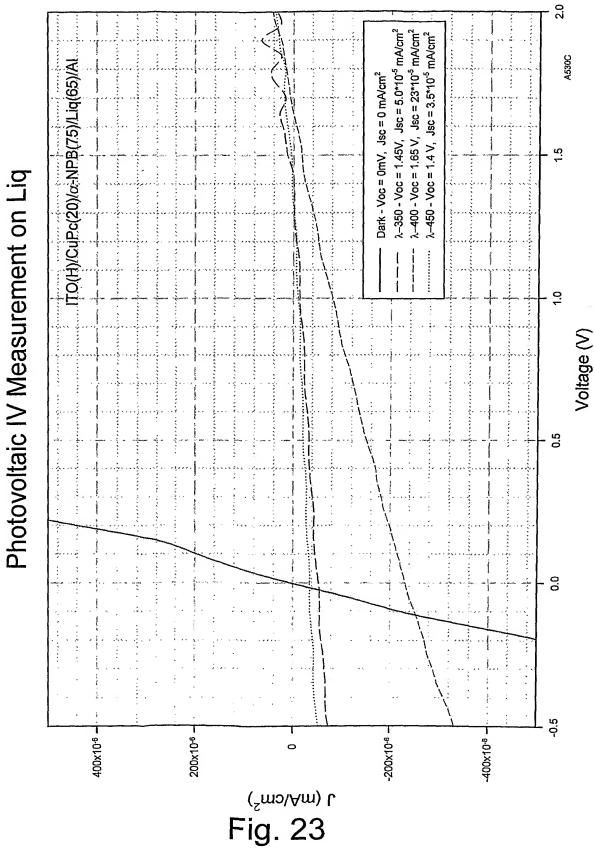
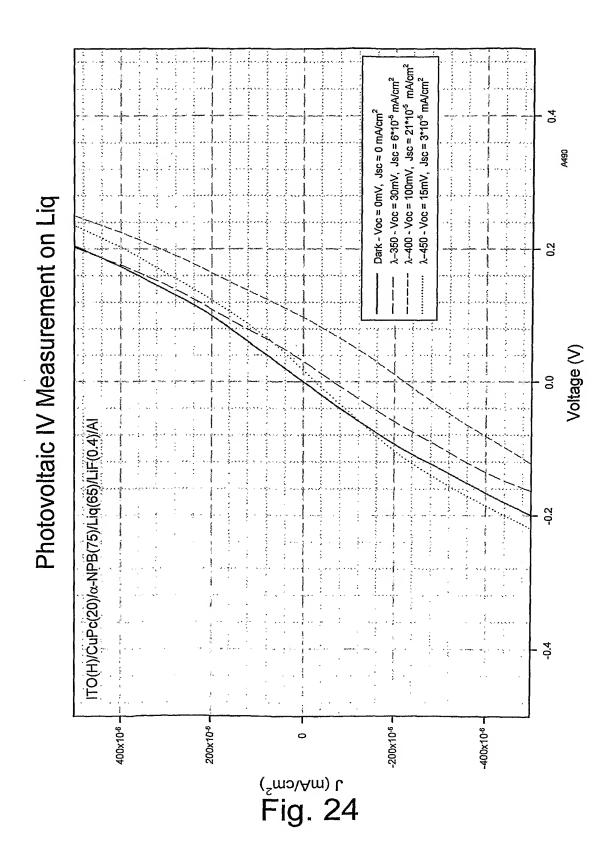


Fig. 21







DERWENT-ACC-NO: 2004-143133

DERWENT-WEEK: 200629

COPYRIGHT 2010 DERWENT INFORMATION LTD

TITLE: Photovoltaic device such as solar

cell, comprises metal chelate as

photovoltaic element

INVENTOR: ANTIPAN-LARA J; KATHIRGAMANATHAN P;

PARTHEEPAN A

PATENT-ASSIGNEE: ELAM LTD[ELAMN]

PRIORITY-DATA: 2002GB-016154 (July 12, 2002)

PATENT-FAMILY:

PUB-NO	PUB-DATE	LANGUAGE
WO 2004008554 .	A2 January 22,	2004 EN
AU 2003281003	A1 February 2,	2004 EN
AU 2003281003 .	A8 November 3,	2005 EN

DESIGNATED-STATES: AE AG AL AM AT AU AZ BA BB BG

BR BY BZ CA CH CN CO CR CU CZ
DE DK DM DZ EC EE ES FI GB GD
GE GH GM HR HU ID IL IN IS JP
KE KG KP KR KZ LC LK LR LS LT
LU LV MA MD MG MK MN MW MX MZ

NO NZ OM PH PL PT RO RU SD SE S

G SK SL TJ TM TN TR TT TZ UA UG

US UZ VN YU ZA ZM ZW AT BE BG CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IT KE LS LU

MC MW MZ NL OA PT RO SD SE SI

SK SL SZ TR TZ UG ZM ZW

APPLICATION-DATA:

PUB-NO	APPL-DESCRIPTOR	APPL-NO	APPL- DATE
WO2004008554A2	N/A	2003WO- GB03035	July 14, 2003
AU2003281003A1	N/A	2003AU- 281003	July 14, 2003
AU2003281003A8	Based on	2003AU- 281003	July 14, 2003

INT-CL-CURRENT:

TYPE	IPC DATE	
CIPS	H01L51/00	20060101
CIPS	H01L51/30	20060101

ABSTRACTED-PUB-NO: WO 2004008554 A2

BASIC-ABSTRACT:

NOVELTY - The photovoltaic device comprises metal chelate (3-12) as photovoltaic element.

USE - Photovoltaic cells such as solar cells for converting solar radiation into usable electrical energy.

ADVANTAGE - The metal chelates absorbs light of

specific wavelength(s) depending on metal and ligands used. The photocurrent output of solar cell is maximized by increasing total number of photons of different energy and wavelength. A wide range of visible spectrum can be obtained by providing several layers of different metal chelate which absorb light of different wavelengths. The metal chelates also absorbs light in infrared, ultraviolet or shorter wavelengths, thereby improving utilization of sunlight and increasing power achievable by solar cell.

DESCRIPTION OF DRAWING(S) — The graph shows the relationship of voltage and current measured when photovoltaic device is exposed to light of various wavelengths.

EQUIVALENT-ABSTRACTS:

ORGANIC CHEMISTRY

Preferred Device: The photovoltaic device comprises a first electrode comprising a metal, the photovoltaic element and second electrode, provided sequentially. The second electrode is a transparent substrate which is a conductive glass or plastic material and covers at least a portion of photovoltaic element.

Preferred Element: The photovoltaic element comprises organometallic complex of formula (1) or (2) or binuclear, trinuclear, or polynuclear organometallic complexes of formulae (3-12).

(Lalpha) nM (1a)

(Lalpha) nM-Lp (Ib)

```
M = rare earth, non-rare earth, transition,
lanthanide or actinide metals preferably samarium
(III), europium (II), europium (III), terbium
(III), dysprosium (III), ytterbium (III), lutetium
(III), gadolinium (III), uranium (III), thulium
(III), cerium (III), praseodymium (III), neodymium
(III), promethium (III), holmium (III) and erbium
(III) or lithium, sodium, potassium, rubidium,
cesium, beryllium, magnesium, calcium, strontium,
barium, copper, silver, gold, zinc, cadmium, boron,
aluminum, gallium, indium, germanium, tin,
antimony, manganese, iron, ruthenium, osmium,
cobalt, nickel, palladium, platinum, cadmium,
chromium, titanium, vanadium, zirconium, tantalum,
molybdenum, rhodium, iridium, titanium, niobium,
scandium or yttrium, lead;
n = valency of M;
Lalpha and Lp = organic ligands.
(Ln)nM1M2 (2a)
(Ln) nM1M2 (Lp) (2b)
Ln = Lalpha;
Lp = neutral ligand;
M1 = rare earth, transition metal, lanthanide or
actinide;
M2 = non-rare earth metal;
n = valency of M1 and M2.
(Lm) \times M1 - M2 (Ln) y (3)
```

```
L = bridging ligand;
M1 = rare earth metal;
M2 = M1 or non-rare earth metal;
Lm, Ln = Lalpha;
x = valency of M1;
y = valency of M2.
(Lm) \times M1 - M3 (Ln) y - M2 (Lp) z (5)
M1, M2, M3 = same or different rare earth metal;
Lp = Lalpha;
z = valency of M3.
M1-M2-M3-M4 (9)
M1-M2-M4-M3 (10)
M4 = M1; and
```

L = bridging ligand, where rare earth and non-rare earth metal are joined by metal to metal bond and/ or via an intermediate bridging atom such that ligand or molecular group of more than 3 metals are joined by metal to metal bond and/or via intermediate ligands.

The organic metallic chelate is a metal quinolate preferably lithium quinolate, aluminum quinolate, scandium quinolate, zirconium quinolate, hafnium quinolate or vanadium quinolate, doped with

fluorescent, phosphorescent or ion fluorescent compound. The dopant is preferably diphenylquinacridine, diphenylquinacridone, coumarins, perylene or their derivatives. The photovoltaic element preferably has structure of formula (IA).

M = M1; and

R1-R3 = H, optionally substituted hydrocarbyl, aliphatic groups, aromatic groups, heterocyclic and polycyclic ring structures, fluorocarbons and trifluoromethyl, halogens and thiophenyl groups.

A photovoltaic device was fabricated on a clean and dried ITO (indium tin oxide) coated glass piece by sequentially forming layers by vacuum evaporation to form a structure, ITO/CuPc(20 nm)/TPD(50 nm)/Eu (DBM)3(OPNP)/85 nm Alq3/LiF(0.4 nm)/Al, where CuPc is copper phthalocyanine, TPD is N, N'-diphenyl-N, N'-bis (3-methylphenyl)-1,1' -biphenyl -4,4' diamine, Alq3 is aluminum quinolate, LiF is lithium fluoride and Al is aluminum. The organic coating on the portion etched with concentrated hydrochloric acid was wiped with a cotton bud. The coated electrodes were stored in a vacuum desiccator over a molecular sieve and phosphorous pentoxide, until they were loaded into a vacuum coater and contacted with aluminum top. The active area of the photovoltaic device was 0.08 cm by 0.1 cm2. The devices were then kept in a vacuum desiccator and photovoltaic studies were performed. The device was connected to an electric circuit and exposed to light of various wavelengths and the voltage and current were measured. The results were shown graphically where the open circuit voltage Voc and short circuit current Jsc were plotted.

CHOSEN-DRAWING: Dwg.21/24

TITLE-TERMS: PHOTOVOLTAIC DEVICE SOLAR CELL

COMPRISE METAL CHELATE ELEMENT

DERWENT-CLASS: E11 E12 L03 U11 U12 X15

CPI-CODES: E05-A; E05-B; E05-C; E05-D; E05-F;

E05-G; E05-J; E05-K; E05-L; E05-M;

E05-N; E05-P; E05-Q; L03-E05B;

EPI-CODES: U11-A01X; U12-A02A2X;

CHEMICAL-CODES: Chemical Indexing M3 *01*

Fragmentation Code A103 A960 C710

D021 D621 H4 H401 H441 H8 M280

M320 M411 M511 M520 M530 M540 M630

M781 Q454 R043 Specific Compounds

RA22LX Registry Numbers 300121

Chemical Indexing M3 *02*

Fragmentation Code A313 A960 C710

D021 D621 H4 H401 H441 H8 M280

M320 M411 M511 M520 M530 M540 M630

M781 Q454 R043 Specific Compounds

R20372 RA2QMS Registry Numbers

134570 14922 332819

Chemical Indexing M3 *03*

Fragmentation Code A421 A960 C710

D021 D621 H4 H401 H441 H8 M280

M320 M411 M511 M520 M530 M540 M630

M781 Q454 R043 Specific Compounds

mior 2434 Mo43 Specific compounds

RA1YYH Registry Numbers 295190

Chemical Indexing M3 *04*

Fragmentation Code A540 A960 C710

D021 D621 H4 H401 H441 H8 M280

M320 M411 M511 M520 M530 M540 M630

M781 Q454 R043 Specific Compounds

RA1YYI Registry Numbers 295191

Chemical Indexing M3 *05*
Fragmentation Code A672 A960 C710
D021 D621 H4 H401 H441 H8 M280
M320 M411 M511 M520 M530 M540 M630
M781 Q454 R043 Specific Compounds
RACAHJ Registry Numbers 806835

Chemical Indexing M3 *06*
Fragmentation Code A765 A960 B515
B701 B720 B730 B731 B744 B815 B832
C710 G010 G019 G100 J582 M121 M129
M144 M148 M149 M210 M214 M233 M262
M280 M282 M311 M320 M321 M342 M382
M391 M411 M510 M520 M530 M533 M540
M620 M630 M781 Q454 R043 Specific
Compounds RA0480 Registry Numbers
205837

Chemical Indexing M3 *07*
Fragmentation Code A765 A960 A970
B605 B720 B732 B770 B803 B831 C710
F011 F019 F511 F599 H213 J582 M210
M211 M262 M280 M282 M311 M320 M321
M342 M382 M391 M411 M510 M520 M523
M530 M540 M620 M630 M781 Q454 R043
Specific Compounds RAD3HF Registry
Numbers 845952

Chemical Indexing M3 *08*
Fragmentation Code A677 A923 A960
F011 F012 F013 F014 F015 F019 F431
F499 F512 G010 G011 G019 G100 H211
J521 J581 L941 M113 M119 M121 M144
M210 M211 M215 M233 M240 M262 M280
M281 M320 M411 M510 M521 M522 M531
M532 M540 M630 M650 M781 Q454 R043

Specific Compounds RAD3HH Registry Numbers 845954

Chemical Indexing M3 *09* Fragmentation Code A103 A111 A119 A137 A155 A204 A212 A220 A238 A256 A400 A429 A500 A547 A600 A679 A700 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A892 A940 A960 A970 B115 B134 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B815 B831 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C803 C804 C805 C806 C807 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E600 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H211 H401 H402 H441 H442 H521 H541 H542 H543 H581 H582 H583 H601 H607 H608 H609 H621 H641 H642 H643 H681 H682 H683 H685 H689 H715 H721 H722 J011 J012 J013 J111 J112 J131 J132 J133 J151 J171 J172 J173 J211 J241 J242 J271 J272 J411 J471 J472 J490 J521 J581 J582 J598 J599 K130 K199 K352 K399 K442 K499 K810 K830 K850 K899 L145 L352 L353 L355 L399 L410 L420 L431 L499 L512 L531 L532 L560 L599 L650 L941 L999 M111 M112 M113 M114 M115 M116 M119 M121 M122 M123 M124 M125 M126 M129 M131 M135 M136 M139 M141 M143 M144 M147 M148 M149 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M280 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M340 M342 M343 M344 M349 M382 M391 M392 M393 M411 M510 M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M620 M630 M781 Q454 R043 Markush Compounds 012117301

Chemical Indexing M3 *10*
Fragmentation Code A313 A331 A332
A349 A350 A351 A382 A421 A422 A423
A424 A425 A426 A427 A428 A430 A539

A424 A425 A426 A427 A428 A430 A539 A540 A541 A542 A544 A545 A546 A548 A673 A676 A677 A678 A940 A960 A970 B115 B134 B305 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B809 B815 B831 B832 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C803 C804 C805 C806 C807 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E600 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H211 H401 H402 H441 H442 H521 H541 H542 H543 H581 H582 H583 H601 H607 H608 H609 H621 H641 H642 H643 H681 H682 H683 H685 H689 H715 H721 H722 J011 J012 J013 J111

J112 J131 J132 J133 J151 J171 J172 J173 J211 J241 J242 J271 J272 J411

J471 J472 J490 J521 J581 J582 J598 J599 K130 K199 K352 K399 K442 K499 K810 K830 K850 K899 L145 L352 L353 L355 L399 L410 L420 L431 L499 L512 L531 L532 L560 L599 L650 L941 L999 M111 M112 M113 M114 M115 M116 M119 M121 M122 M123 M124 M125 M126 M129 M131 M135 M136 M139 M141 M143 M144 M147 M148 M149 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M280 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M340 M342 M343 M344 M349 M382 M391 M392 M393 M411 M510 M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M620 M630 M781 Q454 R043 Markush Compounds 012117302

Chemical Indexing M3 *11*

Fragmentation Code A103 A111 A119 A137 A155 A204 A212 A220 A238 A256 A400 A429 A500 A547 A600 A679 A700 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A892 A940 A960 A970 B215 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B730 B731 B732 B741 B742 B743 B744 B751 B752 B760 B770 B791 B799 B803 B815 B832 B833 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C804 C805 C806 C807 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 F610 F699 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020

```
G021 G022 G029 G030 G040 G050 G100
G111 G112 G113 G221 G299 G553 G563
H100 H101 H102 H103 H141 H142 H143
H211 H212 H401 H402 H441 H442 H521
H541 H542 H543 H581 H582 H583 H600
H601 H607 H608 H609 H621 H641 H642
H643 H681 H682 H683 H685 H689 H715
H721 H722 H723 J011 J012 J013 J111
J112 J131 J132 J133 J151 J171 J172
J173 J211 J241 J242 J271 J272 J411
J471 J472 J490 J521 J522 J581 J582
J598 J599 K130 K199 K352 K399 K442
K499 K810 K830 K850 K899 L145 L352
L353 L355 L399 L410 L420 L431 L499
L512 L531 L532 L560 L599 L650 L922
L941 L999 M111 M112 M113 M114 M115
M116 M119 M121 M122 M123 M124 M125
M126 M129 M131 M135 M136 M139 M141
M143 M144 M147 M148 M149 M150 M210
M211 M212 M213 M214 M215 M216 M220
M221 M222 M223 M224 M225 M226 M231
M232 M233 M280 M311 M312 M313 M314
M315 M316 M320 M321 M322 M323 M331
M332 M333 M340 M342 M343 M344 M349
M382 M391 M392 M393 M411 M510 M511
M512 M513 M520 M521 M522 M523 M530
M531 M532 M533 M540 M541 M620 M630
M781 Q454 R043 Markush Compounds
012117303
```

Chemical Indexing M3 *12*
Fragmentation Code A313 A331 A332
A349 A350 A351 A382 A421 A422 A423
A424 A425 A426 A427 A428 A430 A539
A540 A541 A542 A544 A545 A546 A548
A673 A676 A677 A678 A940 A960 A970
B215 B305 B415 B434 B505 B515 B534
B605 B615 B634 B701 B711 B712 B713

```
B720 B730 B731 B732 B741 B742 B743
B744 B751 B752 B760 B770 B791 B799
B803 B809 B815 B832 B833 B834 C000
C101 C106 C107 C108 C116 C216 C316
C710 C800 C801 C802 C804 C805 C806
C807 D010 D011 D012 D013 D019 D020
D021 D022 D029 D040 D049 D621 D622
E600 F010 F011 F012 F013 F014 F015
F019 F020 F021 F029 F211 F512 F610
F699 G001 G002 G010 G011 G012 G013
G014 G015 G016 G019 G020 G021 G022
G029 G030 G040 G050 G100 G111 G112
G113 G221 G299 G553 G563 H100 H101
H102 H103 H141 H142 H143 H211 H212
H401 H402 H441 H442 H521 H541 H542
H543 H581 H582 H583 H600 H601 H607
H608 H609 H621 H641 H642 H643 H681
H682 H683 H685 H689 H715 H721 H722
H723 J011 J012 J013 J111 J112 J131
J132 J133 J151 J171 J172 J173 J211
J241 J242 J271 J272 J411 J471 J472
J490 J521 J522 J581 J582 J598 J599
K130 K199 K352 K399 K442 K499 K810
K830 K850 K899 L145 L352 L353 L355
L399 L410 L420 L431 L499 L512 L531
L532 L560 L599 L650 L922 L941 L999
M111 M112 M113 M114 M115 M116 M119
M121 M122 M123 M124 M125 M126 M129
M131 M135 M136 M139 M141 M143 M144
M147 M148 M149 M150 M210 M211 M212
M213 M214 M215 M216 M220 M221 M222
M223 M224 M225 M226 M231 M232 M233
M280 M311 M312 M313 M314 M315 M316
M320 M321 M322 M323 M331 M332 M333
M340 M342 M343 M344 M349 M382 M391
M392 M393 M411 M510 M511 M512 M513
M520 M521 M522 M523 M530 M531 M532
M533 M540 M541 M620 M630 M781 Q454
```

R043 Markush Compounds 012117304

Chemical Indexing M3 *13* Fragmentation Code A103 A111 A119 A137 A155 A204 A212 A220 A238 A256 A400 A429 A500 A547 A600 A679 A700 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A892 A940 A960 A970 B215 B415 B434 B505 B515 B534 B605 B615 B634 B701 B702 B711 B712 B713 B720 B721 B722 B732 B741 B742 B744 B751 B752 B760 B770 B791 B798 B799 B803 B815 B832 B833 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C720 C800 C801 C802 C803 C804 C805 C806 C807 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H211 H401 H402 H441 H442 H521 H541 H542 H543 H581 H582 H583 H600 H601 H607 H608 H609 H621 H641 H642 H643 H681 H682 H683 H685 H689 H715 H721 H722 H723 J011 J012 J013 J111 J112 J131 J132 J133 J151 J171 J172 J173 J211 J241 J242 J271 J272 J411 J471 J472 J490 J521 J581 J582 J598 J599 K130 K199 K352 K399 K442 K499 K810 K830 K850 K899 L145 L352 L353 L355 L399 L410 L420 L431 L499 L512 L531 L532 L560 L599 L650 L941 L999 M111 M112 M113 M114 M115 M116 M119 M121 M122 M123 M124 M125 M126 M129 M131 M135 M136 M139 M141 M143 M144 M147 M148 M149 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M280 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M340 M342 M343 M344 M349 M382 M391 M392 M393 M411 M510 M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M620 M630 M781 Q454 R043 Markush Compounds 012117305

Chemical Indexing M3 *14*

Fragmentation Code A313 A331 A332 A349 A350 A351 A382 A421 A422 A423 A424 A425 A426 A427 A428 A430 A539 A540 A541 A542 A544 A545 A546 A548 A673 A676 A677 A678 A940 A960 A970 B215 B305 B415 B434 B505 B515 B534 B605 B615 B634 B701 B702 B711 B712 B713 B720 B721 B722 B732 B741 B742 B744 B751 B752 B760 B770 B791 B798 B799 B803 B809 B815 B832 B833 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C720 C800 C801 C802 C803 C804 C805 C806 C807 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H211 H401 H402 H441 H442 H521 H541 H542 H543 H581 H582 H583 H600 H601 H607 H608 H609 H621 H641 H642 H643 H681 H682 H683 H685 H689 H715 H721 H722 H723 J011 J012

J013 J111 J112 J131 J132 J133 J151 J171 J172 J173 J211 J241 J242 J271 J272 J411 J471 J472 J490 J521 J581 J582 J598 J599 K130 K199 K352 K399 K442 K499 K810 K830 K850 K899 L145 L352 L353 L355 L399 L410 L420 L431 L499 L512 L531 L532 L560 L599 L650 L941 L999 M111 M112 M113 M114 M115 M116 M119 M121 M122 M123 M124 M125 M126 M129 M131 M135 M136 M139 M141 M143 M144 M147 M148 M149 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M280 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M340 M342 M343 M344 M349 M382 M391 M392 M393 M411 M510 M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M620 M630 M781 Q454 R043 Markush Compounds 012117306

Chemical Indexing M3 *15* Fragmentation Code A103 A111 A119 A137 A155 A204 A212 A220 A238 A256 A400 A429 A500 A547 A600 A679 A700 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A892 A940 A960 A970 B215 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B815 B831 B832 B833 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C720 C800 C801 C802 C803 C804 C805 C806 C807 D000 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E160 E220 E600 F010 F011 F012

```
F013 F014 F015 F019 F020 F021 F029
F211 F512 G000 G001 G002 G010 G011
G012 G013 G014 G015 G016 G019 G020
G021 G022 G029 G030 G040 G050 G100
G111 G112 G113 G221 G299 G341 G553
G563 H100 H101 H141 H142 H211 H401
H402 H441 H442 H521 H541 H542 H543
H581 H582 H583 H600 H601 H607 H608
H609 H621 H622 H641 H642 H643 H681
H682 H683 H685 H689 H715 H721 H722
H723 J011 J012 J013 J111 J112 J131
J132 J133 J151 J171 J172 J173 J211
J241 J242 J271 J272 J411 J471 J472
J490 J521 J581 J582 J598 J599 K130
K199 K352 K399 K442 K499 K810 K830
K850 K899 L145 L352 L353 L355 L399
L410 L420 L431 L499 L512 L531 L532
L560 L599 L650 L941 L999 M111 M112
M113 M114 M115 M116 M119 M121 M122
M123 M124 M125 M126 M129 M131 M135
M136 M139 M141 M143 M144 M147 M148
M149 M150 M210 M211 M212 M213 M214
M215 M216 M220 M221 M222 M223 M224
M225 M226 M231 M232 M233 M280 M311
M312 M313 M314 M315 M316 M320 M321
M322 M323 M331 M332 M333 M340 M342
M343 M344 M349 M382 M391 M392 M393
M411 M510 M511 M512 M513 M520 M521
M522 M523 M530 M531 M532 M533 M540
M541 M620 M630 M781 Q454 R043 Ring
Index Numbers 03480 03524 Markush
Compounds 012117307
```

Chemical Indexing M3 *16*
Fragmentation Code A313 A331 A332
A349 A350 A351 A382 A421 A422 A423
A424 A425 A426 A427 A428 A430 A539
A540 A541 A542 A544 A545 A546 A548

```
A673 A676 A677 A678 A940 A960 A970
B215 B305 B415 B434 B505 B515 B534
B605 B615 B634 B701 B711 B712 B713
B720 B741 B742 B751 B752 B760 B770
B791 B799 B803 B809 B815 B831 B832
B833 B834 C000 C101 C106 C107 C108
C116 C216 C316 C710 C720 C800 C801
C802 C803 C804 C805 C806 C807 D000
D010 D011 D012 D013 D019 D020 D021
D022 D029 D040 D049 D621 D622 E160
E220 E600 F010 F011 F012 F013 F014
F015 F019 F020 F021 F029 F211 F512
G000 G001 G002 G010 G011 G012 G013
G014 G015 G016 G019 G020 G021 G022
G029 G030 G040 G050 G100 G111 G112
G113 G221 G299 G341 G553 G563 H100
H101 H141 H142 H211 H401 H402 H441
H442 H521 H541 H542 H543 H581 H582
H583 H600 H601 H607 H608 H609 H621
H622 H641 H642 H643 H681 H682 H683
H685 H689 H715 H721 H722 H723 J011
J012 J013 J111 J112 J131 J132 J133
J151 J171 J172 J173 J211 J241 J242
J271 J272 J411 J471 J472 J490 J521
J581 J582 J598 J599 K130 K199 K352
K399 K442 K499 K810 K830 K850 K899
L145 L352 L353 L355 L399 L410 L420
L431 L499 L512 L531 L532 L560 L599
L650 L941 L999 M111 M112 M113 M114
M115 M116 M119 M121 M122 M123 M124
M125 M126 M129 M131 M135 M136 M139
M141 M143 M144 M147 M148 M149 M150
M210 M211 M212 M213 M214 M215 M216
M220 M221 M222 M223 M224 M225 M226
M231 M232 M233 M280 M311 M312 M313
M314 M315 M316 M320 M321 M322 M323
M331 M332 M333 M340 M342 M343 M344
M349 M382 M391 M392 M393 M411 M510
```

M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M620 M630 M781 Q454 R043 Ring Index Numbers 03480 03524 Markush Compounds 012117308

Chemical Indexing M3 *17* Fragmentation Code A103 A111 A119 A137 A155 A204 A212 A220 A238 A256 A400 A429 A500 A547 A600 A679 A700 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A892 A940 A960 A970 B215 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B815 B831 C000 C101 C106 C107 C108 C116 C216 C316 C710 C720 C800 C801 C802 C803 C804 C805 C806 C807 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E600 F010 F011 F012 F013 F014 F015 F016 F019 F020 F021 F029 F211 F431 F499 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H211 H401 H402 H441 H442 H521 H541 H542 H543 H581 H582 H583 H600 H601 H607 H608 H609 H621 H622 H623 H641 H642 H643 H681 H682 H683 H685 H689 H715 H721 H722 H723 J011 J012 J013 J111 J112 J131 J132 J133 J151 J171 J172 J173 J211 J241 J242 J271 J272 J411 J471 J472 J490 J521 J581 J582 J598 J599 K130 K199 K352 K399 K442 K499 K810 K830 K850 K899 L145 L352 L353 L355 L399 L410 L420 L431 L499

L512 L531 L532 L560 L599 L650 L941 L999 M111 M112 M113 M114 M115 M116 M119 M121 M122 M123 M124 M125 M126 M129 M131 M135 M136 M139 M141 M143 M144 M147 M148 M149 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M280 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M340 M342 M343 M344 M349 M382 M391 M392 M393 M411 M510 M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M532 M533 M540 M541 M620 M630 M781 Q454 R043 Markush Compounds 012117309

Chemical Indexing M3 *18* Fragmentation Code A313 A331 A332 A349 A350 A351 A382 A421 A422 A423 A424 A425 A426 A427 A428 A430 A539 A540 A541 A542 A544 A545 A546 A548 A673 A676 A677 A678 A940 A960 A970 B215 B305 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B809 B815 B831 B832 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C720 C800 C801 C802 C803 C804 C805 C806 C807 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E600 F010 F011 F012 F013 F014 F015 F016 F019 F020 F021 F029 F211 F431 F499 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142

H211 H401 H402 H441 H442 H521 H541

```
H542 H543 H581 H582 H583 H600 H601
H607 H608 H609 H621 H622 H623 H641
H642 H643 H681 H682 H683 H685 H689
H715 H721 H722 H723 J011 J012 J013
J111 J112 J131 J132 J133 J151 J171
J172 J173 J211 J241 J242 J271 J272
J411 J471 J472 J490 J521 J581 J582
J598 J599 K130 K199 K352 K399 K442
K499 K810 K830 K850 K899 L145 L352
L353 L355 L399 L410 L420 L431 L499
L512 L531 L532 L560 L599 L650 L941
L999 M111 M112 M113 M114 M115 M116
M119 M121 M122 M123 M124 M125 M126
M129 M131 M135 M136 M139 M141 M143
M144 M147 M148 M149 M150 M210 M211
M212 M213 M214 M215 M216 M220 M221
M222 M223 M224 M225 M226 M231 M232
M233 M280 M311 M312 M313 M314 M315
M316 M320 M321 M322 M323 M331 M332
M333 M340 M342 M343 M344 M349 M382
M391 M392 M393 M411 M510 M511 M512
M513 M520 M521 M522 M523 M530 M531
M532 M533 M540 M541 M620 M630 M781
Q454 R043 Markush Compounds
012117310
```

Chemical Indexing M3 *19* Fragmentation Code A103 A111 A119 A137 A155 A204 A212 A220 A238 A256 A400 A429 A500 A547 A600 A679 A700 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A892 A940 A960 A970 B215 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B815 B831 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C804

```
C805 C806 C807 D010 D011 D012 D013
D014 D019 D020 D021 D022 D029 D040
D049 D621 D622 E350 E600 F010 F011
F012 F013 F014 F015 F019 F020 F021
F029 F211 F512 G001 G002 G010 G011
G012 G013 G014 G015 G016 G019 G020
G021 G022 G029 G030 G040 G050 G100
G111 G112 G113 G221 G299 G553 G563
H100 H101 H103 H141 H142 H211 H212
H401 H402 H441 H442 H521 H541 H542
H543 H581 H582 H583 H600 H601 H607
H608 H609 H621 H641 H642 H643 H681
H682 H683 H685 H689 H715 H721 H722
H723 J011 J012 J013 J111 J112 J131
J132 J133 J151 J171 J172 J173 J211
J241 J242 J271 J272 J411 J471 J472
J490 J521 J523 J581 J582 J598 J599
K130 K199 K352 K399 K442 K499 K810
K830 K850 K899 L145 L352 L353 L355
L399 L410 L420 L431 L499 L512 L531
L532 L560 L599 L650 L930 L941 L999
M111 M112 M113 M114 M115 M116 M119
M121 M122 M123 M124 M125 M126 M129
M131 M135 M136 M139 M141 M143 M144
M147 M148 M149 M150 M210 M211 M212
M213 M214 M215 M216 M220 M221 M222
M223 M224 M225 M226 M231 M232 M233
M280 M311 M312 M313 M314 M315 M316
M320 M321 M322 M323 M331 M332 M333
M340 M342 M343 M344 M349 M382 M391
M392 M393 M411 M510 M511 M512 M513
M520 M521 M522 M523 M530 M531 M532
M533 M540 M541 M620 M630 M781 Q454
R043 Ring Index Numbers 07309
Markush Compounds 012117311
```

Chemical Indexing M3 *20*
Fragmentation Code A313 A331 A332

```
A349 A350 A351 A382 A421 A422 A423
A424 A425 A426 A427 A428 A430 A539
A540 A541 A542 A544 A545 A546 A548
A673 A676 A677 A678 A940 A960 A970
B215 B305 B415 B434 B505 B515 B534
B605 B615 B634 B701 B711 B712 B713
B720 B741 B742 B751 B752 B760 B770
B791 B799 B803 B809 B815 B831 B832
B834 C000 C101 C106 C107 C108 C116
C216 C316 C710 C800 C801 C802 C804
C805 C806 C807 D010 D011 D012 D013
D014 D019 D020 D021 D022 D029 D040
D049 D621 D622 E350 E600 F010 F011
F012 F013 F014 F015 F019 F020 F021
F029 F211 F512 G001 G002 G010 G011
G012 G013 G014 G015 G016 G019 G020
G021 G022 G029 G030 G040 G050 G100
G111 G112 G113 G221 G299 G553 G563
H100 H101 H103 H141 H142 H211 H212
H401 H402 H441 H442 H521 H541 H542
H543 H581 H582 H583 H600 H601 H607
H608 H609 H621 H641 H642 H643 H681
H682 H683 H685 H689 H715 H721 H722
H723 J011 J012 J013 J111 J112 J131
J132 J133 J151 J171 J172 J173 J211
J241 J242 J271 J272 J411 J471 J472
J490 J521 J523 J581 J582 J598 J599
K130 K199 K352 K399 K442 K499 K810
K830 K850 K899 L145 L352 L353 L355
L399 L410 L420 L431 L499 L512 L531
L532 L560 L599 L650 L930 L941 L999
M111 M112 M113 M114 M115 M116 M119
M121 M122 M123 M124 M125 M126 M129
M131 M135 M136 M139 M141 M143 M144
M147 M148 M149 M150 M210 M211 M212
M213 M214 M215 M216 M220 M221 M222
M223 M224 M225 M226 M231 M232 M233
M280 M311 M312 M313 M314 M315 M316
```

M320 M321 M322 M323 M331 M332 M333 M340 M342 M343 M344 M349 M382 M391 M392 M393 M411 M510 M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M620 M630 M781 Q454 R043 Ring Index Numbers 07309 Markush Compounds 012117312

Chemical Indexing M3 *21* Fragmentation Code A103 A111 A119 A137 A155 A204 A212 A220 A238 A256 A400 A429 A500 A547 A600 A679 A700 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A892 A940 A960 A970 B215 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B815 B831 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C804 C805 C806 C807 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E100 E199 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H103 H141 H142 H201 H202 H211 H401 H402 H441 H442 H521 H541 H542 H543 H581 H582 H583 H600 H601 H607 H608 H609 H621 H641 H642 H643 H681 H682 H683 H685 H689 H715 H721 H722 H723 J011 J012 J013 J111 J112 J131 J132 J133 J151 J171 J172 J173 J211 J241 J242 J271 J272 J411 J471 J472 J490 J521 J581 J582 J598 J599 K130 K199 K352 K399 K442 K499 K810

```
K830 K850 K899 L145 L352 L353 L355
L399 L410 L420 L431 L499 L512 L531
L532 L560 L599 L650 L941 L999 M111
M112 M113 M114 M115 M116 M119 M121
M122 M123 M124 M125 M126 M129 M131
M132 M133 M135 M136 M139 M141 M143
M144 M147 M148 M149 M150 M210 M211
M212 M213 M214 M215 M216 M220 M221
M222 M223 M224 M225 M226 M231 M232
M233 M280 M311 M312 M313 M314 M315
M316 M320 M321 M322 M323 M331 M332
M333 M340 M342 M343 M344 M349 M382
M391 M392 M393 M411 M510 M511 M512
M513 M520 M521 M522 M523 M530 M531
M532 M533 M540 M541 M610 M620 M630
M781 Q454 R043 Markush Compounds
012117313
```

Chemical Indexing M3 *22* Fragmentation Code A313 A331 A332 A349 A350 A351 A382 A421 A422 A423 A424 A425 A426 A427 A428 A430 A539 A540 A541 A542 A544 A545 A546 A548 A673 A676 A677 A678 A940 A960 A970 B215 B305 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B809 B815 B831 B832 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C804 C805 C806 C807 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E100 E199 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563

```
H100 H101 H103 H141 H142 H201 H202
H211 H401 H402 H441 H442 H521 H541
H542 H543 H581 H582 H583 H600 H601
H607 H608 H609 H621 H641 H642 H643
H681 H682 H683 H685 H689 H715 H721
H722 H723 J011 J012 J013 J111 J112
J131 J132 J133 J151 J171 J172 J173
J211 J241 J242 J271 J272 J411 J471
J472 J490 J521 J581 J582 J598 J599
K130 K199 K352 K399 K442 K499 K810
K830 K850 K899 L145 L352 L353 L355
L399 L410 L420 L431 L499 L512 L531
L532 L560 L599 L650 L941 L999 M111
M112 M113 M114 M115 M116 M119 M121
M122 M123 M124 M125 M126 M129 M131
M132 M133 M135 M136 M139 M141 M143
M144 M147 M148 M149 M150 M210 M211
M212 M213 M214 M215 M216 M220 M221
M222 M223 M224 M225 M226 M231 M232
M233 M280 M311 M312 M313 M314 M315
M316 M320 M321 M322 M323 M331 M332
M333 M340 M342 M343 M344 M349 M382
M391 M392 M393 M411 M510 M511 M512
M513 M520 M521 M522 M523 M530 M531
M532 M533 M540 M541 M610 M620 M630
M781 Q454 R043 Markush Compounds
012117314
```

Chemical Indexing M3 *23*
Fragmentation Code A103 A111 A119
A137 A155 A204 A212 A220 A238 A256
A400 A429 A500 A547 A600 A679 A700
A758 A759 A760 A761 A762 A763 A764
A765 A766 A767 A768 A769 A770 A771
A892 A940 A960 A970 B215 B415 B434
B505 B515 B534 B605 B615 B634 B701
B711 B712 B713 B720 B741 B742 B751
B752 B760 B770 B791 B799 B803 B815

```
B831 C000 C101 C106 C107 C108 C116
C216 C316 C710 C800 C801 C802 C804
C805 C806 C807 D000 D010 D011 D012
D013 D014 D015 D019 D020 D021 D022
D029 D040 D049 D621 D622 E350 E600
F010 F011 F012 F013 F014 F015 F019
F020 F021 F029 F211 F512 G001 G002
G010 G011 G012 G013 G014 G015 G016
G019 G020 G021 G022 G029 G030 G040
G050 G100 G111 G112 G113 G221 G299
G553 G563 H100 H101 H141 H142 H211
H401 H402 H441 H442 H521 H541 H542
H543 H581 H582 H583 H600 H601 H607
H608 H609 H621 H622 H623 H641 H642
H643 H681 H682 H683 H685 H689 H715
H721 H722 H723 J011 J012 J013 J111
J112 J131 J132 J133 J151 J171 J172
J173 J211 J241 J242 J271 J272 J411
J471 J472 J490 J521 J581 J582 J598
J599 K130 K199 K352 K399 K442 K499
K810 K830 K850 K899 L145 L352 L353
L355 L399 L410 L420 L431 L499 L512
L531 L532 L560 L599 L650 L941 L999
M111 M112 M113 M114 M115 M116 M119
M121 M122 M123 M124 M125 M126 M129
M131 M135 M136 M139 M141 M143 M144
M147 M148 M149 M150 M210 M211 M212
M213 M214 M215 M216 M220 M221 M222
M223 M224 M225 M226 M231 M232 M233
M280 M311 M312 M313 M314 M315 M316
M320 M321 M322 M323 M331 M332 M333
M340 M342 M343 M344 M349 M382 M391
M392 M393 M411 M510 M511 M512 M513
M520 M521 M522 M523 M530 M531 M532
M533 M540 M541 M620 M630 M781 Q454
R043 Ring Index Numbers 05479
Markush Compounds 012117315
```

Chemical Indexing M3 *24* Fragmentation Code A313 A331 A332 A349 A350 A351 A382 A421 A422 A423 A424 A425 A426 A427 A428 A430 A539 A540 A541 A542 A544 A545 A546 A548 A673 A676 A677 A678 A940 A960 A970 B215 B305 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B809 B815 B831 B832 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C804 C805 C806 C807 D000 D010 D011 D012 D013 D014 D015 D019 D020 D021 D022 D029 D040 D049 D621 D622 E350 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H211 H401 H402 H441 H442 H521 H541 H542 H543 H581 H582 H583 H600 H601 H607 H608 H609 H621 H622 H623 H641 H642 H643 H681 H682 H683 H685 H689 H715 H721 H722 H723 J011 J012 J013 J111 J112 J131 J132 J133 J151 J171 J172 J173 J211 J241 J242 J271 J272 J411 J471 J472 J490 J521 J581 J582 J598 J599 K130 K199 K352 K399 K442 K499 K810 K830 K850 K899 L145 L352 L353 L355 L399 L410 L420 L431 L499 L512 L531 L532 L560 L599 L650 L941 L999 M111 M112 M113 M114 M115 M116 M119 M121 M122 M123 M124 M125 M126 M129 M131 M135 M136 M139 M141 M143 M144 M147 M148 M149 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M280 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M340 M342 M343 M344 M349 M382 M391 M392 M393 M411 M510 M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M620 M630 M781 Q454 R043 Ring Index Numbers 05479 Markush Compounds 012117316

Chemical Indexing M3 *25* Fragmentation Code A103 A111 A119 A137 A155 A204 A212 A220 A238 A256 A400 A422 A423 A429 A500 A547 A600 A679 A700 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A892 A940 A960 A970 B215 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B815 B831 C000 C101 C106 C107 C108 C116 C216 C316 C550 C710 C720 C801 C802 C804 C805 C807 D000 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E350 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H211 H401 H402 H441 H442 H521 H541 H542 H543 H581 H582 H583 H600 H601 H607 H608 H609 H621 H641 H642 H643 H681 H682 H683 H685 H689 H715 H721 H722 J011 J012 J013 J111 J112 J131 J132 J133 J151 J171 J172 J173 J211 J241 J242 J271 J272 J411 J471 J472 J490

```
J521 J581 J582 J598 J599 K130 K199
K352 K399 K442 K499 K810 K830 K850
K899 L145 L352 L353 L355 L399 L410
L420 L431 L499 L512 L531 L532 L560
L599 L650 L941 L999 M111 M112 M113
M114 M115 M116 M119 M121 M122 M123
M124 M125 M126 M129 M131 M135 M136
M139 M141 M143 M144 M147 M148 M149
M150 M210 M211 M212 M213 M214 M215
M216 M220 M221 M222 M223 M224 M225
M226 M231 M232 M233 M280 M311 M312
M313 M314 M315 M316 M320 M321 M322
M323 M331 M332 M333 M340 M342 M343
M344 M349 M382 M391 M392 M393 M411
M510 M511 M512 M513 M520 M521 M522
M523 M530 M531 M532 M533 M540 M541
M620 M630 M781 Q454 R043 Ring
Index Numbers 07541 Markush
Compounds 012117317
```

Chemical Indexing M3 *26* Fragmentation Code A313 A331 A332 A349 A350 A351 A382 A421 A422 A423 A424 A425 A426 A427 A428 A430 A539 A540 A541 A542 A544 A545 A546 A548 A673 A676 A677 A678 A940 A960 A970 B215 B305 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B809 B815 B831 B832 B834 C000 C101 C106 C107 C108 C116 C216 C316 C550 C710 C720 C801 C802 C804 C805 C807 D000 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E350 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020

```
G021 G022 G029 G030 G040 G050 G100
G111 G112 G113 G221 G299 G553 G563
H100 H101 H141 H142 H211 H401 H402
H441 H442 H521 H541 H542 H543 H581
H582 H583 H600 H601 H607 H608 H609
H621 H641 H642 H643 H681 H682 H683
H685 H689 H715 H721 H722 J011 J012
J013 J111 J112 J131 J132 J133 J151
J171 J172 J173 J211 J241 J242 J271
J272 J411 J471 J472 J490 J521 J581
J582 J598 J599 K130 K199 K352 K399
K442 K499 K810 K830 K850 K899 L145
L352 L353 L355 L399 L410 L420 L431
L499 L512 L531 L532 L560 L599 L650
L941 L999 M111 M112 M113 M114 M115
M116 M119 M121 M122 M123 M124 M125
M126 M129 M131 M135 M136 M139 M141
M143 M144 M147 M148 M149 M150 M210
M211 M212 M213 M214 M215 M216 M220
M221 M222 M223 M224 M225 M226 M231
M232 M233 M280 M311 M312 M313 M314
M315 M316 M320 M321 M322 M323 M331
M332 M333 M340 M342 M343 M344 M349
M382 M391 M392 M393 M411 M510 M511
M512 M513 M520 M521 M522 M523 M530
M531 M532 M533 M540 M541 M620 M630
M781 Q454 R043 Ring Index Numbers
07541 Markush Compounds 012117318
```

Chemical Indexing M3 *27*
Fragmentation Code A103 A111 A119
A137 A155 A204 A212 A220 A238 A256
A400 A429 A500 A547 A600 A679 A700
A758 A759 A760 A761 A762 A763 A764
A765 A766 A767 A768 A769 A770 A771
A892 A940 A960 A970 B215 B415 B434
B505 B515 B534 B605 B615 B634 B701
B711 B712 B713 B720 B741 B742 B751

```
B752 B760 B770 B791 B799 B803 B815
B831 C000 C101 C106 C107 C108 C116
C216 C316 C710 C800 C801 C802 C804
C805 C806 C807 D010 D011 D012 D013
D019 D020 D021 D022 D029 D040 D049
D621 D622 E600 F010 F011 F012 F013
F014 F015 F019 F020 F021 F029 F211
F512 G001 G002 G010 G011 G012 G013
G014 G015 G016 G019 G020 G021 G022
G029 G030 G040 G050 G100 G111 G112
G113 G221 G299 G553 G563 H100 H101
H103 H141 H142 H143 H211 H401 H402
H441 H442 H521 H541 H542 H543 H581
H582 H583 H600 H601 H607 H608 H609
H621 H641 H642 H643 H681 H682 H683
H685 H689 H715 H721 H722 H723 J011
J012 J013 J111 J112 J131 J132 J133
J151 J171 J172 J173 J211 J241 J242
J271 J272 J411 J471 J472 J490 J521
J581 J582 J598 J599 K130 K199 K352
K399 K442 K499 K810 K830 K850 K899
L145 L352 L353 L355 L399 L410 L420
L431 L499 L512 L531 L532 L560 L599
L650 L941 L999 M111 M112 M113 M114
M115 M116 M119 M121 M122 M123 M124
M125 M126 M129 M131 M135 M136 M139
M141 M143 M144 M147 M148 M149 M150
M210 M211 M212 M213 M214 M215 M216
M220 M221 M222 M223 M224 M225 M226
M231 M232 M233 M280 M311 M312 M313
M314 M315 M316 M320 M321 M322 M323
M331 M332 M333 M340 M342 M343 M344
M349 M382 M391 M392 M393 M411 M510
M511 M512 M513 M520 M521 M522 M523
M530 M531 M532 M533 M540 M541 M620
M630 M781 Q454 R043 Markush
Compounds 012117319
```

Chemical Indexing M3 *28* Fragmentation Code A313 A331 A332 A349 A350 A351 A382 A421 A422 A423 A424 A425 A426 A427 A428 A430 A539 A540 A541 A542 A544 A545 A546 A548 A673 A676 A677 A678 A940 A960 A970 B215 B305 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B809 B815 B831 B832 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C804 C805 C806 C807 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H103 H141 H142 H143 H211 H401 H402 H441 H442 H521 H541 H542 H543 H581 H582 H583 H600 H601 H607 H608 H609 H621 H641 H642 H643 H681 H682 H683 H685 H689 H715 H721 H722 H723 J011 J012 J013 J111 J112 J131 J132 J133 J151 J171 J172 J173 J211 J241 J242 J271 J272 J411 J471 J472 J490 J521 J581 J582 J598 J599 K130 K199 K352 K399 K442 K499 K810 K830 K850 K899 L145 L352 L353 L355 L399 L410 L420 L431 L499 L512 L531 L532 L560 L599 L650 L941 L999 M111 M112 M113 M114 M115 M116 M119 M121 M122 M123 M124 M125 M126 M129 M131 M135 M136 M139 M141 M143 M144 M147 M148 M149 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226

```
M231 M232 M233 M280 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M340 M342 M343 M344 M349 M382 M391 M392 M393 M411 M510 M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M620 M630 M781 Q454 R043 Markush Compounds 012117320
```

Chemical Indexing M3 *29* Fragmentation Code A103 A111 A119 A137 A155 A204 A212 A220 A238 A256 A400 A429 A500 A547 A600 A679 A700 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A892 A940 A960 A970 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B743 B751 B760 B770 B791 B799 B803 B815 B831 B832 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C804 C805 C806 C807 D000 D011 D012 D013 D021 D022 D023 D029 D621 D622 E100 E600 F011 F012 F013 F014 F015 F211 F512 G001 G002 G020 G021 G022 G029 G031 G038 G039 G040 G041 G050 G310 G399 G553 G563 H100 H101 H102 H103 H121 H141 H142 H143 H181 H201 H211 H401 H402 H441 H442 H521 H541 H542 H543 H581 H582 H583 H600 H601 H607 H608 H609 H621 H622 H641 H642 H643 H681 H682 H683 H685 H689 H713 H715 H716 H721 H722 H723 J011 J012 J013 J111 J112 J131 J132 J133 J151 J171 J172 J173 J211 J241 J242 J271 J272 J411 J471 J472 J490 J521 J581 J582 J598 J599 K130 K199 K352 K399 K441 K442 K499 K810 K830 K850 K899

L145 L352 L353 L355 L399 L410 L420 L431 L499 L512 L531 L532 L560 L599 L650 L941 L999 M111 M112 M113 M114 M115 M116 M119 M121 M122 M123 M124 M125 M126 M129 M131 M135 M136 M139 M141 M142 M143 M144 M147 M148 M149 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M280 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M340 M342 M343 M344 M349 M382 M391 M392 M393 M411 M510 M511 M520 M521 M530 M531 M532 M540 M620 M630 M781 Q454 R043 Ring Index Numbers 06706 Markush Compounds 012117321

Fragmentation Code A313 A331 A332 A349 A350 A351 A382 A421 A422 A423 A424 A425 A426 A427 A428 A430 A539 A540 A541 A542 A544 A545 A546 A548 A673 A676 A677 A678 A940 A960 A970 B215 B305 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B743 B751 B752 B760 B770 B791 B799 B803 B809 B815 B831 B832 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C804 C805 C806 C807 D000 D011 D012 D013 D021 D022 D023 D029 D621 D622 E100 E600 F011 F012 F013 F014 F015 F211 F512 G001 G002 G020 G021 G022 G029 G031 G038 G039 G040 G041 G050 G310 G399 G553 G563 H100 H101 H102 H103 H121 H141 H142 H143 H181 H201 H211 H401 H402 H441 H442 H521 H541

H542 H543 H581 H582 H583 H600 H601

Chemical Indexing M3 *30*

```
H607 H608 H609 H621 H622 H641 H642
H643 H681 H682 H683 H685 H689 H713
H715 H716 H721 H722 H723 J011 J012
J013 J111 J112 J131 J132 J133 J151
J171 J172 J173 J211 J241 J242 J271
J272 J411 J471 J472 J490 J521 J581
J582 J598 J599 K130 K199 K352 K399
K441 K442 K499 K810 K830 K850 K899
L145 L352 L353 L355 L399 L410 L420
L431 L499 L512 L531 L532 L560 L599
L650 L941 L999 M111 M112 M113 M114
M115 M116 M119 M121 M122 M123 M124
M125 M126 M129 M131 M135 M136 M139
M141 M142 M143 M144 M147 M148 M149
M150 M210 M211 M212 M213 M214 M215
M216 M220 M221 M222 M223 M224 M225
M226 M231 M232 M233 M280 M311 M312
M313 M314 M315 M316 M320 M321 M322
M323 M331 M332 M333 M340 M342 M343
M344 M349 M382 M391 M392 M393 M411
M510 M511 M520 M521 M530 M531 M532
M540 M620 M630 M781 Q454 R043 Ring
Index Numbers 06706 Markush
Compounds 012117322
```

Chemical Indexing M3 *31*
Fragmentation Code A103 A111 A119
A137 A155 A204 A212 A220 A238 A256
A400 A429 A500 A547 A600 A679 A700
A758 A759 A760 A761 A762 A763 A764
A765 A766 A767 A768 A769 A770 A771
A892 A940 A960 A970 B215 B415 B434
B505 B515 B534 B605 B615 B634 B701
B711 B712 B713 B720 B741 B742 B751
B752 B760 B770 B791 B799 B803 B815
B831 C000 C101 C106 C107 C108 C116
C216 C316 C710 C800 C801 C802 C804
C805 C806 C807 D010 D011 D012 D013

```
D019 D020 D021 D022 D029 D040 D049
D621 D622 E600 F010 F011 F012 F013
F014 F015 F019 F020 F021 F029 F211
F512 G001 G002 G010 G011 G012 G013
G014 G015 G016 G019 G020 G021 G022
G029 G030 G040 G050 G100 G111 G112
G113 G221 G299 G331 G399 G553 G563
H100 H101 H141 H142 H211 H401 H402
H441 H442 H521 H541 H542 H543 H581
H582 H583 H600 H601 H607 H608 H609
H621 H641 H642 H643 H681 H682 H683
H685 H689 H713 H715 H716 H721 H722
H723 J011 J012 J013 J111 J112 J131
J132 J133 J151 J171 J172 J173 J211
J241 J242 J271 J272 J411 J471 J472
J490 J521 J581 J582 J598 J599 K122
K130 K199 K352 K399 K442 K499 K810
K830 K850 K899 L145 L352 L353 L355
L399 L410 L420 L431 L499 L512 L531
L532 L560 L599 L650 L941 L999 M111
M112 M113 M114 M115 M116 M119 M121
M122 M123 M124 M125 M126 M129 M131
M132 M135 M136 M139 M141 M142 M143
M144 M147 M148 M149 M150 M210 M211
M212 M213 M214 M215 M216 M220 M221
M222 M223 M224 M225 M226 M231 M232
M233 M280 M311 M312 M313 M314 M315
M316 M320 M321 M322 M323 M331 M332
M333 M334 M340 M342 M343 M344 M349
M382 M391 M392 M393 M411 M510 M511
M512 M513 M520 M521 M522 M523 M530
M531 M532 M533 M540 M541 M620 M630
M781 Q454 R043 Markush Compounds
012117323
```

Chemical Indexing M3 *32*
Fragmentation Code A313 A331 A332
A349 A350 A351 A382 A421 A422 A423

```
A424 A425 A426 A427 A428 A430 A539
A540 A541 A542 A544 A545 A546 A548
A673 A676 A677 A678 A940 A960 A970
B215 B305 B415 B434 B505 B515 B534
B605 B615 B634 B701 B711 B712 B713
B720 B741 B742 B751 B752 B760 B770
B791 B799 B803 B809 B815 B831 B832
B834 C000 C101 C106 C107 C108 C116
C216 C316 C710 C800 C801 C802 C804
C805 C806 C807 D010 D011 D012 D013
D019 D020 D021 D022 D029 D040 D049
D621 D622 E600 F010 F011 F012 F013
F014 F015 F019 F020 F021 F029 F211
F512 G001 G002 G010 G011 G012 G013
G014 G015 G016 G019 G020 G021 G022
G029 G030 G040 G050 G100 G111 G112
G113 G221 G299 G331 G399 G553 G563
H100 H101 H141 H142 H211 H401 H402
H441 H442 H521 H541 H542 H543 H581
H582 H583 H600 H601 H607 H608 H609
H621 H641 H642 H643 H681 H682 H683
H685 H689 H713 H715 H716 H721 H722
H723 J011 J012 J013 J111 J112 J131
J132 J133 J151 J171 J172 J173 J211
J241 J242 J271 J272 J411 J471 J472
J490 J521 J581 J582 J598 J599 K122
K130 K199 K352 K399 K442 K499 K810
K830 K850 K899 L145 L352 L353 L355
L399 L410 L420 L431 L499 L512 L531
L532 L560 L599 L650 L941 L999 M111
M112 M113 M114 M115 M116 M119 M121
M122 M123 M124 M125 M126 M129 M131
M132 M135 M136 M139 M141 M142 M143
M144 M147 M148 M149 M150 M210 M211
M212 M213 M214 M215 M216 M220 M221
M222 M223 M224 M225 M226 M231 M232
M233 M280 M311 M312 M313 M314 M315
M316 M320 M321 M322 M323 M331 M332
```

M333 M334 M340 M342 M343 M344 M349 M382 M391 M392 M393 M411 M510 M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M620 M630 M781 Q454 R043 Markush Compounds 012117324

Chemical Indexing M3 *33* Fragmentation Code A103 A111 A119 A137 A155 A204 A212 A220 A238 A256 A400 A429 A500 A600 A679 A700 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A892 A940 A960 A970 B215 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B730 B741 B742 B743 B751 B752 B760 B770 B791 B799 B803 B815 B831 B832 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C804 C805 C806 C807 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H211 H401 H402 H441 H442 H521 H541 H542 H543 H581 H582 H583 H600 H601 H607 H608 H609 H621 H641 H642 H643 H681 H682 H683 H685 H689 H715 H721 H722 H723 J011 J012 J013 J111 J112 J131 J132 J133 J151 J171 J172 J173 J211 J241 J242 J271 J272 J411 J471 J472 J490 J521 J581 J582 J598 J599 K130 K199 K352 K399 K442 K499 K810 K830 K850 K899 L145 L352 L353 L355 L399 L410 L420 L431 L499 L512 L531 L532 L560
L599 L650 L941 L999 M111 M112 M113
M114 M115 M116 M119 M121 M122 M123
M124 M125 M126 M129 M131 M135 M136
M139 M141 M143 M144 M147 M148 M149
M150 M210 M211 M212 M213 M214 M215
M216 M220 M221 M222 M223 M224 M225
M226 M231 M232 M233 M280 M311 M312
M313 M314 M315 M316 M320 M321 M322
M323 M331 M332 M333 M340 M342 M343
M344 M349 M382 M391 M392 M393 M411
M510 M511 M512 M513 M520 M521 M522
M523 M530 M531 M532 M533 M540 M541
M620 M630 M781 Q454 R043 Markush
Compounds 012117325

Chemical Indexing M3 *34*

Fragmentation Code A313 A331 A332 A349 A350 A351 A382 A421 A422 A423 A424 A425 A426 A427 A428 A430 A539 A540 A541 A542 A544 A545 A546 A548 A673 A676 A677 A678 A940 A960 A970 B215 B305 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B730 B741 B742 B743 B751 B752 B760 B770 B791 B799 B803 B809 B815 B831 B832 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C804 C805 C806 C807 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D621 D622 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H211 H401 H402 H441 H442 H521 H541 H542 H543 H581

```
H582 H583 H600 H601 H607 H608 H609
H621 H641 H642 H643 H681 H682 H683
H685 H689 H715 H721 H722 H723 J011
J012 J013 J111 J112 J131 J132 J133
J151 J171 J172 J173 J211 J241 J242
J271 J272 J411 J471 J472 J490 J521
J581 J582 J598 J599 K130 K199 K352
K399 K442 K499 K810 K830 K850 K899
L145 L352 L353 L355 L399 L410 L420
L431 L499 L512 L531 L532 L560 L599
L650 L941 L999 M111 M112 M113 M114
M115 M116 M119 M121 M122 M123 M124
M125 M126 M129 M131 M135 M136 M139
M141 M143 M144 M147 M148 M149 M150
M210 M211 M212 M213 M214 M215 M216
M220 M221 M222 M223 M224 M225 M226
M231 M232 M233 M280 M311 M312 M313
M314 M315 M316 M320 M321 M322 M323
M331 M332 M333 M340 M342 M343 M344
M349 M382 M391 M392 M393 M411 M510
M511 M512 M513 M520 M521 M522 M523
M530 M531 M532 M533 M540 M541 M620
M630 M781 Q454 R043 Markush
Compounds 012117326
```

Chemical Indexing M3 *35*

Fragmentation Code A103 A111 A119
A137 A155 A204 A212 A220 A238 A256
A400 A429 A500 A547 A600 A679 A700
A758 A759 A760 A761 A762 A763 A764
A765 A766 A767 A768 A769 A770 A771
A892 A940 A960 A970 B215 B415 B434
B505 B515 B534 B605 B615 B634 B701
B711 B712 B713 B720 B741 B742 B751
B752 B760 B770 B791 B799 B803 B815
B831 C000 C101 C106 C107 C108 C116
C216 C316 C710 C800 C801 C802 C804
C805 C806 C807 D000 D010 D011 D012

```
D013 D019 D020 D021 D022 D023 D029
D040 D049 D120 D210 D621 D622 E400
E600 F010 F011 F012 F013 F014 F015
F019 F020 F021 F029 F211 F512 G001
G002 G010 G011 G012 G013 G014 G015
G016 G019 G020 G021 G022 G029 G030
G040 G050 G100 G111 G112 G113 G221
G299 G553 G563 H100 H101 H102 H103
H141 H142 H211 H401 H402 H441 H442
H521 H541 H542 H543 H581 H582 H583
H600 H601 H607 H608 H609 H621 H641
H642 H643 H681 H682 H683 H685 H689
H715 H721 H722 J011 J012 J013 J111
J112 J131 J132 J133 J151 J171 J172
J173 J211 J241 J242 J271 J272 J411
J471 J472 J490 J521 J581 J582 J598
J599 K130 K199 K352 K399 K442 K499
K810 K830 K850 K899 L145 L352 L353
L355 L399 L410 L420 L431 L499 L512
L531 L532 L560 L599 L650 L941 L942
L999 M111 M112 M113 M114 M115 M116
M119 M121 M122 M123 M124 M125 M126
M129 M131 M135 M136 M139 M141 M143
M144 M147 M148 M149 M150 M210 M211
M212 M213 M214 M215 M216 M220 M221
M222 M223 M224 M225 M226 M231 M232
M233 M280 M311 M312 M313 M314 M315
M316 M320 M321 M322 M323 M331 M332
M333 M340 M342 M343 M344 M349 M382
M391 M392 M393 M411 M510 M511 M512
M513 M520 M521 M522 M523 M530 M531
M532 M533 M540 M541 M620 M630 M781
Q454 R043 Markush Compounds
012117327
```

Chemical Indexing M3 *36*
Fragmentation Code A313 A331 A332
A349 A350 A351 A382 A421 A422 A423

```
A424 A425 A426 A427 A428 A430 A539
A540 A541 A542 A544 A545 A546 A548
A673 A676 A677 A678 A940 A960 A970
B215 B305 B415 B434 B505 B515 B534
B605 B615 B634 B701 B711 B712 B713
B720 B741 B742 B751 B752 B760 B770
B791 B799 B803 B809 B815 B831 B832
B834 C000 C101 C106 C107 C108 C116
C216 C316 C710 C800 C801 C802 C804
C805 C806 C807 D000 D010 D011 D012
D013 D019 D020 D021 D022 D023 D029
D040 D049 D120 D210 D621 D622 E400
E600 F010 F011 F012 F013 F014 F015
F019 F020 F021 F029 F211 F512 G001
G002 G010 G011 G012 G013 G014 G015
G016 G019 G020 G021 G022 G029 G030
G040 G050 G100 G111 G112 G113 G221
G299 G553 G563 H100 H101 H102 H103
H141 H142 H211 H401 H402 H441 H442
H521 H541 H542 H543 H581 H582 H583
H600 H601 H607 H608 H609 H621 H641
H642 H643 H681 H682 H683 H685 H689
H715 H721 H722 J011 J012 J013 J111
J112 J131 J132 J133 J151 J171 J172
J173 J211 J241 J242 J271 J272 J411
J471 J472 J490 J521 J581 J582 J598
J599 K130 K199 K352 K399 K442 K499
K810 K830 K850 K899 L145 L352 L353
L355 L399 L410 L420 L431 L499 L512
L531 L532 L560 L599 L650 L941 L942
L999 M111 M112 M113 M114 M115 M116
M119 M121 M122 M123 M124 M125 M126
M129 M131 M135 M136 M139 M141 M143
M144 M147 M148 M149 M150 M210 M211
M212 M213 M214 M215 M216 M220 M221
M222 M223 M224 M225 M226 M231 M232
M233 M280 M311 M312 M313 M314 M315
M316 M320 M321 M322 M323 M331 M332
```

M333 M340 M342 M343 M344 M349 M382 M391 M392 M393 M411 M510 M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M620 M630 M781 Q454 R043 Markush Compounds 012117328

Chemical Indexing M3 *37* Fragmentation Code A103 A111 A119 A137 A155 A204 A212 A220 A238 A256 A400 A429 A500 A547 A600 A679 A700 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A892 A940 A960 A970 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B760 B770 B791 B799 B803 B815 B831 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C804 C805 C806 C807 D010 D011 D012 D013 D014 D019 D020 D021 D022 D029 D040 D049 D621 D622 E250 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H211 H212 H401 H402 H441 H442 H521 H541 H542 H543 H581 H582 H583 H600 H601 H607 H608 H609 H621 H641 H642 H643 H681 H682 H683 H685 H689 H713 H715 H716 H721 H722 J011 J012 J013 J111 J112 J131 J132 J133 J151 J171 J172 J173 J211 J241 J242 J271 J272 J411 J471 J472 J490 J521 J523 J581 J582 J598 J599 K130 K199 K352 K399 K442 K499 K810 K830 K850 K899 L145 L352 L353 L355 L399 L410

L420 L431 L499 L512 L531 L532 L560 L599 L650 L930 L941 L999 M111 M112 M113 M114 M115 M116 M119 M121 M122 M123 M124 M125 M126 M129 M131 M135 M136 M139 M141 M143 M144 M147 M148 M149 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M280 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M340 M342 M343 M344 M349 M382 M391 M392 M393 M411 M510 M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M620 M630 M781 Q454 R043 Ring Index Numbers 02448 Markush Compounds 012117329

Chemical Indexing M3 *38*

Fragmentation Code A313 A331 A332 A349 A350 A351 A382 A421 A422 A423 A424 A425 A426 A427 A428 A430 A539 A540 A541 A542 A544 A545 A546 A548 A673 A676 A677 A678 A940 A960 A970 B215 B305 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B809 B815 B831 B832 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C804 C805 C806 C807 D010 D011 D012 D013 D014 D019 D020 D021 D022 D029 D040 D049 D621 D622 E250 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H211 H212 H401

```
H402 H441 H442 H521 H541 H542 H543
H581 H582 H583 H600 H601 H607 H608
H609 H621 H641 H642 H643 H681 H682
H683 H685 H689 H713 H715 H716 H721
H722 J011 J012 J013 J111 J112 J131
J132 J133 J151 J171 J172 J173 J211
J241 J242 J271 J272 J411 J471 J472
J490 J521 J523 J581 J582 J598 J599
K130 K199 K352 K399 K442 K499 K810
K830 K850 K899 L145 L352 L353 L355
L399 L410 L420 L431 L499 L512 L531
L532 L560 L599 L650 L930 L941 L999
M111 M112 M113 M114 M115 M116 M119
M121 M122 M123 M124 M125 M126 M129
M131 M135 M136 M139 M141 M143 M144
M147 M148 M149 M150 M210 M211 M212
M213 M214 M215 M216 M220 M221 M222
M223 M224 M225 M226 M231 M232 M233
M280 M311 M312 M313 M314 M315 M316
M320 M321 M322 M323 M331 M332 M333
M340 M342 M343 M344 M349 M382 M391
M392 M393 M411 M510 M511 M512 M513
M520 M521 M522 M523 M530 M531 M532
M533 M540 M541 M620 M630 M781 O454
R043 Ring Index Numbers 02448
Markush Compounds 012117330
```

Chemical Indexing M3 *39*
Fragmentation Code A103 A111 A119
A137 A155 A204 A212 A220 A238 A256
A400 A429 A500 A547 A600 A679 A700
A758 A759 A760 A761 A762 A763 A764
A765 A766 A767 A768 A769 A770 A771
A892 A940 A960 A970 B215 B415 B434
B505 B515 B534 B605 B615 B634 B701
B711 B712 B713 B720 B741 B742 B751
B752 B760 B770 B791 B799 B803 B815
B831 C000 C101 C106 C107 C108 C116

```
C216 C316 C710 C800 C801 C802 C804
C805 C806 C807 D010 D011 D012 D013
D019 D020 D021 D022 D029 D040 D049
D420 D621 D622 E600 F010 F011 F012
F013 F014 F015 F019 F020 F021 F029
F211 F512 G001 G002 G010 G011 G012
G013 G014 G015 G016 G019 G020 G021
G022 G029 G030 G040 G050 G100 G111
G112 G113 G221 G299 G553 G563 H100
H101 H141 H142 H211 H401 H402 H441
H442 H521 H541 H542 H543 H581 H582
H583 H600 H601 H607 H608 H609 H621
H641 H642 H643 H681 H682 H683 H685
H689 H715 H721 H722 H723 J011 J012
J013 J111 J112 J131 J132 J133 J151
J171 J172 J173 J211 J241 J242 J271
J272 J411 J471 J472 J490 J521 J581
J582 J598 J599 K130 K199 K352 K399
K441 K442 K499 K810 K830 K850 K899
L145 L352 L353 L355 L399 L410 L420
L431 L499 L512 L531 L532 L560 L599
L650 L941 L999 M111 M112 M113 M114
M115 M116 M119 M121 M122 M123 M124
M125 M126 M129 M131 M135 M136 M139
M141 M143 M144 M147 M148 M149 M150
M210 M211 M212 M213 M214 M215 M216
M220 M221 M222 M223 M224 M225 M226
M231 M232 M233 M280 M311 M312 M313
M314 M315 M316 M320 M321 M322 M323
M331 M332 M333 M340 M342 M343 M344
M349 M382 M391 M392 M393 M411 M510
M511 M512 M513 M520 M521 M522 M523
M530 M531 M532 M533 M540 M541 M620
M630 M781 Q454 R043 Ring Index
Numbers 05974 Markush Compounds
012117331
```

Chemical Indexing M3 *40*

Fragmentation Code A313 A331 A332 A349 A350 A351 A382 A421 A422 A423 A424 A425 A426 A427 A428 A430 A539 A540 A541 A542 A544 A545 A546 A548 A673 A676 A677 A678 A940 A960 A970 B215 B305 B415 B434 B505 B515 B534 B605 B615 B634 B701 B711 B712 B713 B720 B741 B742 B751 B752 B760 B770 B791 B799 B803 B809 B815 B831 B832 B834 C000 C101 C106 C107 C108 C116 C216 C316 C710 C800 C801 C802 C804 C805 C806 C807 D010 D011 D012 D013 D019 D020 D021 D022 D029 D040 D049 D420 D621 D622 E600 F010 F011 F012 F013 F014 F015 F019 F020 F021 F029 F211 F512 G001 G002 G010 G011 G012 G013 G014 G015 G016 G019 G020 G021 G022 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100 H101 H141 H142 H211 H401 H402 H441 H442 H521 H541 H542 H543 H581 H582 H583 H600 H601 H607 H608 H609 H621 H641 H642 H643 H681 H682 H683 H685 H689 H715 H721 H722 H723 J011 J012 J013 J111 J112 J131 J132 J133 J151 J171 J172 J173 J211 J241 J242 J271 J272 J411 J471 J472 J490 J521 J581 J582 J598 J599 K130 K199 K352 K399 K441 K442 K499 K810 K830 K850 K899 L145 L352 L353 L355 L399 L410 L420 L431 L499 L512 L531 L532 L560 L599 L650 L941 L999 M111 M112 M113 M114 M115 M116 M119 M121 M122 M123 M124 M125 M126 M129 M131 M135 M136 M139 M141 M143 M144 M147 M148 M149 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M280 M311 M312 M313

```
M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M340 M342 M343 M344 M349 M382 M391 M392 M393 M411 M510 M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M533 M540 M541 M620 M630 M781 Q454 R043 Ring Index Numbers 05974 Markush Compounds 012117332
```

Chemical Indexing M3 *41* Fragmentation Code A400 A500 A600 A700 A960 A970 B605 B720 B732 B770 B803 B831 C000 C800 C801 C802 C803 C804 C805 C806 C807 D010 D019 D020 D029 D040 D049 F010 F011 F019 F020 F021 F029 F511 F599 G001 G002 G010 G011 G012 G013 G019 G020 G021 G022 G029 G040 G100 G111 G112 G221 G299 H213 H600 H601 H608 H609 H681 H682 H683 H689 J471 J472 J581 J582 L512 L599 M121 M122 M123 M124 M125 M126 M129 M135 M139 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M262 M280 M281 M282 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M340 M342 M343 M349 M362 M372 M382 M391 M392 M393 M411 M510 M511 M512 M513 M520 M521 M522 M523 M530 M531 M532 M533 M540 M620 M630 M781 Q454 R043 Markush Compounds 012117333

UNLINKED-DERWENT-REGISTRY-NUMBERS: ; 1164U

SECONDARY-ACC-NO:

CPI Secondary Accession Numbers: 2004-057734

Non-CPI Secondary Accession Numbers: 2004-114077